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Multivalue Methods

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MULTIVALUE METHODS

by

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Clayton V. Henrie

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CHAPTER I

INTRODUCTION

Methods of solving ordinary differential equations with initial conditions are of a great importance to engineers and scientists. Many of these equations can be solved by well-known analytical techniques, but a greater number of physically significant differential equations cannot be so solved. Thus, the solutions of these equations must be approximated numerically. It is the purpose of this paper to investigate the techniques used in solving differential equations with initial conditions by "multivalue methods."

An nth order ordinary differential equation of the form

$$y^{(n)}(t) = f(y, y', \ldots, y^{(n-1)}(t), t)$$

having the initial conditions

$$y(t_o) = p_o$$

$$y'(t_o) = p_1$$

$$\cdot$$

$$\cdot$$

$$\cdot$$

$$y^{(n-1)}(t_o) = p_{n-1}$$

can be reduced to a system of first-order equations (see Moursand and Duris [4, p. 225])

$$
\begin{aligned}
y_1' &= y_2 & y_1(t_o) &= p_o \\
y_2' &= y_3 & y_2(t_o) &= p_1 \\
&\cdot & &\cdot \\
&\cdot & &\cdot \\
&\cdot & &\cdot \\
y_{n-1}' &= y_n & y_{n-1}(t_o) &= p_{n-1} \\
y_n' &= f(y_1, y_2, \ldots, y_n, t) & y_n(t_o) &= p_{n-1}
\end{aligned}
$$

Since results for first order equations are generalizations of a single first-order equation, we will only consider the problem of finding a numerical approximation for the solution of the single first-order differential equation

$$y' = f(y, t) \tag{1.1}$$

with the initial condition

$$y(0) = y_o$$

on the interval $[0, b]$.

To insure existence and uniqueness of the solution of (1.1), it will be required that $f(y, t)$ be continuous in y and t and satisfies a

Lipschitz condition in y over $[0, b]$. The following theorem (see Gear [1, p. 4]) gives conditions for existence and uniqueness:

Theorem 1.1

If $y' = f(y, t)$ is a differential equation such that $f(y, t)$ is continuous in the region $0 \leq t \leq b$, and if there exists a constant L such that

$$\left| f(y, t) - f(y^*, t) \right| \leq L \left| y - y^* \right|$$

for all $0 \leq t \leq b$ and all y, y^* (this is called the Lipschitz condition and L is called the Lipschitz constant), then there exists a unique continuously differentiable function $y(t)$ such that

$$y'(t) = f(y(t), t) \tag{1.2}$$

and $y(0) = y_o$, the initial condition.

If $\partial f / \partial y$ exists, then the Lipschitz condition guarantees that $\left|\partial f / \partial y\right| \leq L$. Conversely, if f is differentiable with respect to y, and $\left|\partial f / \partial y\right| \leq L$, then f satisfies the Lipschitz condition. Thus, finding a bound on $\partial f / \partial y$ is a way of verifying that a Lipschitz constant exists. It will be assumed throughout this paper that the conditions of Theorem 1.1 are satisfied.

The problems that will be considered will not only have unique solutions, but the problems will also be "well-posed." By this is meant that small perturbations in the stated problem will only lead to small changes in the answers. This is a useful condition because a numerical approximation to the solution may well introduce perturbations and it is desired that the perturbed solution remain close to the true solution; it is desirable that the numerical solution can be made close to the true solution by keeping these perturbations small. In this paper "well-posed" will be defined as follows (see Gear [1, p. 7]):

Definition 1.1

The ordinary differential equation (1.2) is well-posed with respect to the initial condition y_o if there exist strictly positive constants k and ϵ^* such that for any $\epsilon \leq \epsilon^*$ the perturbed problem

$$z' = f(z, t) + \delta(t)$$

$$z(0) = y_o + \epsilon_o$$

satisfies

$$\left| z(t) - y(t) \right| \leq k \epsilon$$

whenever $\left|\epsilon_o\right| \leq \epsilon$, $\left|\delta(t)\right| < \epsilon$ for all $0 \leq t \leq b$ where $\delta(t)$ and ϵ_o are small perturbations.

We state without proof (see Gear [1, p. 7]):

Theorem 1.2

If f(y, t) satisfies a Lipschitz condition, then (1.2) is well-posed with respect to any initial condition.

The numerical techniques to be considered will approximate the solution of the differential equation at a discrete set of evenly spaced points in the interval. To do this we first divide the interval $[0, b]$ into N parts of width $h = b/N$. The points will be denoted $t_n = nh$, $n = 0, 1, 2, \ldots, N$. The notation $y(t_n)$ will denote the exact solution of the differential equation at the point t_n and y_n will be the numerical approximation of the differential equation at t_n.

To construct formulas, we first convert the differential equation to the equivalent integral equation

$$y(t) = y_o + \int_o^t f(y, t)dt, \quad t \epsilon \; [0, b].$$

Let us assume that the exact solution of the differential equation is known at $t_o, t_1, \ldots, t_{n-1}$. From the above integral equation $y(t_n)$ can be written as

$$y(t_n) = y(t_k) + \int_{t_k}^{t_n} f(y, t)dt \tag{1.3}$$

where $0 \le k \le n$. The value $y(t_n)$ can now be approximated with a numerical quadrature formula which approximates the integral in Equation (1.3) by using values of $y(t)$ and $y'(t)$ at some or all of the back points t_i, $i = 0, 1, \ldots, n-1$.

To illustrate the above paragraph, we can approximate the integral in Equation (1.3) by using the quadrature formula

$$\int_{t_{n-1}}^{t_n} f(y,t)dt = \frac{h}{12}\left[23y'(t_{n-1}) - 16y'(t_{n-2}) + 5y'(t_{n-3})\right] - \frac{9}{24}h^4 y^{(4)}(\xi)$$

where

$$\min(t_{n-3}, t_{n-2}, t_{n-1}, t) < \xi < \max(t_{n-3}, t_{n-2}, t_{n-1}, t).$$

Thus, Equation (1.3) becomes

$$y(t_n) = y(t_{n-1}) + \frac{h}{12}\left[23y'(t_{n-1}) - 16y'(t_{n-2}) + 5y'(t_{n-3})\right]$$

$$- \frac{9}{24} h^4 y^{(4)}(\xi). \tag{1.4}$$

Then the numerical approximation y_n to $y(t_n)$ will be

$$y_n = y_{n-1} + \frac{h}{12}\left[23y'_{n-1} - 16y'_{n-2} + 5y'_{n-3}\right] \tag{1.5}$$

where $y'_i = f(y_i, t_i)$. The remainder term $\frac{9}{24} h^4 y^{(4)}(\xi)$ in Equation (1.4) is called the local truncation error. It is the error produced in the single calculation of $y(t_n)$ when using the numerical quadrature formula with exact data.

In general, the local truncation error will be denoted by $0(h^r)$, r an integer, which displays the power of h in the error term. By the notation big 0 of h^r [$0(h^r)$] we mean any function of h such that there exist constants h_o and k independent of h for which

$$\left|0(h^r)\right| \leq kh^r$$

for all $|h| \leq h_o$. If $y^{(4)}(t)$ in Equation (1.4) is continuous on $[0, b]$ (a closed region), then let

$$k_1 = \max\left|y^{(4)}(t)\right|, \quad t \in [0, b].$$

So the remainder term in Equation (1.4) can be written as $0(h^4)$ since

$$\left| 0(h^4) \right| = \frac{9}{24} h^4 \left| y^{(4)}(\xi) \right|$$

$$\leq \frac{9}{24} h^4 k_1$$

$$= kh^4$$

where $k = \frac{9}{24} k_1$. In this paper, a method whose error term is $0(h^{r+1})$ will be said to be of order r (this will be formally defined in Chapter 3). It will be assumed in this paper that $r \geq 0$. Equation (1.4) is a method of order three (Equation (1.4) is the third order Adams-Bashforth method). It will be derived in Chapter 2.

Since y_n is computed in terms of y and y' at the three back points t_{n-i}, i = 1, 2, 3, Equation (1.5) will be called a multivalue method. The general multivalue method to be considered is written as

$$\sum_{i=0}^{k} \alpha_i y_{n-i} = h \sum_{i=0}^{k} \beta_i y'_{n-i}, \quad n = 0, 1, \ldots, N, \qquad (1.6)$$

$\alpha_o \neq 0$, for the initial conditions

$$y_c = y_{o,c}, \quad c = 0, 1, \ldots, k-1$$

where the α_i and β_i are real constants. The notation $y_{o,c}$, $c = 0, 1, \ldots, k-1$ denotes a set of constants which represent the values of y and y' at the back points t_c, $c = 0, 1, \ldots, k-1$.

There are two problems that must be dealt with in using multivalue methods to solve (1.1). First the multivalue method does not give the exact values of the solution of the differential equation because of truncation error; and secondly, numbers cannot be represented exactly in the computer performing the numerical approximation since the computer carries only finite precision arithmetic (errors introduced by this mechanism will be called "round-off error"). Consequently, the solution will be represented by a finite number of finite precision numbers containing two sources of error: 1) local truncation errors due to mathematical approximations made by the multivalue method, and 2) round-off errors the machine makes because it does not carry infinite precision arithmetic.

After a multivalue method has been chosen, it is desired that the method will converge in some sense to the actual solution of(1.1). But it has already been seen that multivalue methods do not give the exact values of the differential equation because of the $0(h^r)$ term being truncated. But we can make the truncation error approach zero by making h small, that is, $0(h^r) \rightarrow 0$ as $h \rightarrow 0$. But, by doing this the number of points in the interval increases. Since the computer carries finite precision arithmetic, the accumulative round-off error (round-off error present in the final result of numerical computation) increases. Thus, we must be careful not to make h too small. In defining convergence of a multivalue method in this paper, it will be assumed that the computations indicated in the method be performed exactly (thus causing no round-off error). Hence, convergence of a multivalue method will be loosely defined to mean that any desired degree of accuracy can be achieved in solving (1.1) numerically by picking a small enough h.

We now need to know that small changes in the initial values of (1.1) only produce bounded changes in the numerical approximations provided by the multivalue method chosen. This concept will be called stability. Stability for multivalue methods is defined as (see Gear [1, p. 9]) follows:

Definition 1.2

If there exists an $h_o > 0$ for each differential equation (1.1) such that a change in the starting values by a fixed amount produces a bounded change in the numerical solution for all $0 < h \leq h_o$, then the method is stable.

Note that the stability does not require convergence, although the converse is true. For example, the "method" $y_n = y_{n-1}$, $n = 1, 2, \ldots, N$ is stable, but not convergent for any differential equation but $y' = 0$.

The concepts of stability of a multivalue method and convergence of the numerical approximation to the actual solution are concerned with the limiting process as $h \to 0$. In practice, we must compute with a finite number of steps where $0 < h \leq h_o$ and are really concerned with the size of errors for such h. In particular, it is desired to know if the errors introduced at each step (truncation and round-off) have a small or large effect on the approximate solution. Therefore, "absolute stability" (see Gear [1, p. 9]) of a multivalue method is defined as follows:

Definition 1.3

A multivalue method is absolutely stable for a given step size h and a given differential equation (1.1) if the change due to a perturbation of size δ in one of the mesh values y_i is no larger than δ in all subsequent values y_n, $n > i$.

The stability of the method is dependent on the differential equation. In this paper the "test equation"

$$y' = \lambda y \qquad (1.7)$$

where λ is a constant, will be considered. (The solution of (1.7) is $y = ce^{\lambda t}$, c a constant. If $\lambda \leq 0$, small perturbations to $ce^{\lambda t}$ lead to small changes in the answers for all $t \in [0, b]$. If $\lambda > 0$, small perturbations to $ce^{\lambda t}$ lead to large changes in the answers, but these changes stay bounded on the interval $[0, b]$). Therefore, absolute stability (see Gear [1, p. 9]) for a multivalue method used in solving (1.7) is defined as:

Definition 1.4

The region of absolute stability for a multivalue method is that set of values of h (real and nonnegative) and λ for which a perturbation in a single value y_i will produce a change in subsequent values which does not increase from step to step.

A multivalue method consists of two processes called prediction and correction. The prediction process is an "explicit multivalue method" which provides an explicit way of computing y_n and hy'_n from the values of y and its derivative at preceding points. The general form of a predictor multivalue method to be discussed in this paper is

$$y_{n,(o)} = \sum_{i=1}^{k} (\alpha_i y_{n-i} + \beta_i h y'_{n-i}) \qquad (1.8)$$

$$hy'_{n-i} = hf(y_{n-i}, t_{n-i}), \; i = 1, 2, \ldots, k$$

where the α_i and β_i are real constants. The notation $y_{n,(o)}$ will be used to denote the predicted value of y_n. Since (1.8) expresses y_n [$y_{n,(o)}$] in terms of information at the k back points $t_{n-1}, t_{n-2}, \ldots, t_{n-k}$ (note that this involves an extrapolation process), it will be referred to as k-step predictor multivalue method.

The corrector process is an "implicit multivalue method" which now uses the differential equation to correct the approximate values found from the predictor if they do not satisfy the differential equation at $t = t_n$. The general form of a corrector multivalue method to be considered in this paper is

$$y_n = \sum_{i=1}^{k} (\alpha_i^* y_{n-i} + \beta_i^* hy'_{n-i}) + \beta_o^* hf(y_{n,(o)}, t_n) \qquad (1.9)$$

$$hy'_{n-i} = hf(y_{n-i}, t_{n-i}), \; i = 1, 2, \ldots, k$$

where the α_i^* and β_i^* are real constants. Since it also uses the information at the k back points $t_{n-1}, t_{n-2}, \ldots, t_{n-k}$, Equation (1.9) will be referred to as a k-step corrector multivalue method. (Equation (1.9) is implicit since it is not possible to solve explicitly for y_n.) The predicted value of y_n $[y_{n,(o)}]$ that was found from the predictor (1.8) is now used in (1.9) which involves an interpolation process to find the new or corrected value of y_n. An example of a corrector multivalue method is

$$y_n = y_{n-1} + \frac{h}{24}(9f(y_n, t_n) + 19y'_{n-1} - 5y'_{n-2} + y'_{n-3}) \qquad (1.10)$$

where $y_i' = f(y_i, t_i)$. This is the Adams-Moulton 3-step multivalue method of order four. Thus, in solving (1.1), (1.8) can be used to predict the solution y(t) and (1.9) to correct the predicted value. Several iterations of (1.9) can then be performed to improve the approximation to y(t). If we let $y_{n,(m)}$ be the value of y_n after the mth iteration of the corrector, then (1.9) can be written as

$$y_{n,(m+1)} = \sum_{i=1}^{k} (\alpha_i^* y_{n-i} + \beta_i^* h y'_{n-i}) + \beta_o^* h f(y_{n,(m)}, t_n)$$

$$y'_{n-i} = f(y_{n-i}, t_{n-i}), \quad i = 1, 2, \ldots, k.$$

CHAPTER II

PREDICTOR-CORRECTOR METHODS

Let Y_{n-1} denote the column vector

$$\left[y_{n-1}, y_{n-2}, \ldots, y_{n-k}, hy'_{n-1}, hy'_{n-2}, \ldots, hy'_{n-k}\right]^T$$

where the y are numerical approximations to the solution of Equation (1.1) at the points t_{n-i}, $i = 1, 2, \ldots, k$ and the y' are numerical approximations to the value of the differential equation at the points t_{n-i}, $i = 1, 2, \ldots, k$. The objective of a multivalue method is to find a numerical approximation for Y_n from Y_{n-1} and the differential equation, where Y_n is the column vector

$$\left[y_n, y_{n-1}, \ldots, y_{n-k+1}, hy'_n, hy'_{n-1}, \ldots, hy'_{n-k+1}\right]^T.$$

Once Y_o is given, this process can then be applied repetitively to compute $Y_1, Y_2, Y_3, \ldots, Y_N$. It is assumed that Y_o is known.

There are two processes involved in using a multivalue method to find a numerical approximation for Y_n from Y_{n-1} and the differential equation. First, the prediction process of a multivalue method approximates Y_n from Y_{n-1} by extrapolation. This approximation will be called $Y_{n,(o)}$ and is given by

$$Y_{n,(o)} = BY_{n-1} \tag{2.1}$$

where $Y_{n,(o)}$ is the column vector

$$\left[y_{n,(o)}, y_{n-1}, \ldots, y_{n-k+1}, hy'_{n,(o)}, hy'_{n-1}, \ldots, hy'_{n-k+1}\right]^T$$

(note that $hy'_{n,(o)}$ denotes the predicted value of hy'_n found from some multivalue method) and B is any suitable matrix of constants. For example, it could be

$$\begin{bmatrix} y_{n,(o)} \\ y_{n-1} \\ \vdots \\ y_{n-k+1} \\ hy'_{n,(o)} \\ hy'_{n-1} \\ \vdots \\ hy'_{n-k+1} \end{bmatrix} = \left[\begin{array}{cccc:cccc} \alpha_1 & \alpha_2 & \cdots & \alpha_k & \beta_1 & \beta_2 & \cdots & \beta_k \\ 1 & & \bigcirc & & & & & \\ & \ddots & & & & \bigcirc & & \\ \bigcirc & & 1 & 0 & & & & \\ \hdashline \gamma_1 & \gamma_2 & \cdots & \gamma_k & \delta_1 & \delta_2 & \cdots & \delta_k \\ & & & & 1 & & \bigcirc & \\ & \bigcirc & & & & \ddots & & \\ & & & & \bigcirc & & 1 & 0 \end{array}\right] \begin{bmatrix} y_{n-1} \\ y_{n-2} \\ \vdots \\ y_{n-k} \\ hy'_{n-1} \\ hy'_{n-2} \\ \vdots \\ hy'_{n-k} \end{bmatrix} \tag{2.2}$$

where the α_i, β_i, γ_i, and δ_i are constants such that

$$\sum_{i=1}^{k} (\alpha_i y_{n-i} + \beta_i hy'_{n-i})$$

is an approximation to y_n (denoted by $y_{n,(o)}$), and

$$\sum_{i=1}^{k} (\alpha_i y_{n-i} + \delta_i hy'_{n-i})$$

is an approximation to hy'_n (denoted by $hy'_{n,(o)}$). Thus, by picking B this way, we are not only predicting the value of y_n, but also hy'_n in terms of y and its derivative at the back points t_{n-i}, $i = 1, 2, \ldots, k$ by extrapolation.

The second process, which is the corrector process, is now used to correct the approximate values so that they satisfy the differential equation at $t = t_n$. The differential equation will be written as

$$\begin{aligned} 0 &= G(Y_n) \\ &= -(Y_n)_k + hf((Y_n)_o) \\ &= -hy'_n = hf(y_n) \end{aligned}$$

where by $(Y)_i$ we mean the ith component of the vector Y (vector component numbering starts from 0) and $f(y_n) = f(y_n, t_n)$. It tells us the amount by which Y_n does not satisfy the differential equation. Hence, the amount by which $Y_{n,(o)}$ does not satisfy the differential equation is $G(Y_{n,(o)})$. This scalar is multiplied by some column vector K and the results is added to $Y_{n,(o)}$ to correct it by the process

$$Y_{n,(1)} = Y_{n,(o)} + KG(Y_{n,(o)}). \tag{2.3}$$

This process can be repeated by

$$Y_{n,(m+1)} = Y_{n,(m)} + KG(Y_{n,(m)}), \tag{2.4}$$

$m = 1, 2, \ldots$ for a fixed number of iterations or until there is no further change in $Y_{n,(m)}$ (note for example that K could be the column vector $K = [0, \ldots, 0, 1, 0, \ldots, 0]^T$ where the 1 appears in the kth position and

$$Y_{n,(j)} = \left[y_{n,(j)}, y_{n-1}, \ldots, hy'_{n,(j)}, hy'_{n-1}, \ldots, hy'_{n-k+1} \right]^T$$

where $y_{n,(j)}$ and $y'_{n,(j)}$ are the corrected values of y_n and y'_n respectively after the jth correction). The value used for Y_n is then $Y_{n,(M)}$ where M is either fixed or large enough to get convergence, that is, such that

$G(Y_{n,(M)})$ is zero to the accuracy desired. We say that M is the number of corrector iterations.

Suppose that B has the form given in (2. 2) with $\gamma_i = \delta_i = 0$, $1 \le i \le k$, and the vector k to be zero in all positions except for the kth, where we place a one. After multiplying Y_{n-1} by B, (2. 1) becomes

$$y_{n,(o)} = \sum_{i=1}^{k} (\alpha_i \, y_{n-i} + \beta_1 \, hy'_{n-i})$$

for the first component and

$$hy'_{n,(o)} = 0$$

for the kth component. Now, $hy'_{n,(1)}$ is the kth component of $Y_{n,(1)}$. Therefore,

$$hy'_{n,(1)} = hf(y_{n,(o)}).$$

Thus, additional iterations of (2. 4) have no further effect, so we can take M = 1 and get

$$y_n = \sum_{i=1}^{k} (\alpha_i y_{n-i} + \beta_i hy'_{n-i})$$

where

$$hy'_{n-i} = hf(y_{n-i}) \quad i = 1, 2, \ldots, k.$$

This is the k-step explicit predictor multivalue method defined by (1.8). Thus, our notation allows for both predictor and corrector multivalue methods.

Equation (1.5) is an example of a 3-step explicit predictor multivalue method. A technique for deriving it is that of undetermined coefficients. A form for the method is assumed, say

$$y_n = \alpha_1 y_{n-1} + h\beta_1 y'_{n-1} + h\beta_2 y'_{n-2} + h\beta_3 y'_{n-3}. \tag{2.5}$$

The α and β are chosen so that the value of y_n computed from (2.5) using correct values for y_{n-1}, y'_{n-1}, y'_{n-2}, and y'_{n-3} differ as little as possible from the true solution. In this case we would like the error to be $0(h^4)$ since (1.5) is of order three (this is the highest possible order one can expect as will be shown below). So we expand $y(t_{n-1})$, $y'(t_{n-2})$, and $y'(t_{n-3})$ by Taylor's formula about t_n with $0(h^4)$ remainders. Since $t_{n-q} = t_n - qh$, then

$$y(t_n) = \alpha_1 y(t_n - h) + \beta_1 hy'(t_n - h) + \beta_2 hy'(t_n - 2h) + \beta_3 hy'(t_n - 3h) + 0(h^4)$$

$$= \alpha_1 \left[y(t_n) - hy'(t_n) + \frac{h^2}{2} y''(t_n) - \frac{h^3}{6} y'''(t_n) + 0(h^4) \right]$$

$$+ \beta_1 \left[hy'(t_n) - h^2 y''(t_n) + \frac{h^3}{2} y'''(t_n) + 0(h^4) \right]$$

$$+ \beta_2 \left[hy'(t_n) - 2h^2 y''(t_n) + 2h^3 y'''(t_n) + 0(h^4) \right]$$

$$+ \beta_3 \left[hy'(t_n) - 3h^2 y''(t_n) + \frac{9}{2} h^3 y'''(t_n) + 0(h^4) \right] .$$

Equating terms in h^0, h^1, h^2, and h^3 on both sides of the equality sign, we get

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 1 & 1 \\ \frac{1}{2} & -1 & -2 & -3 \\ \frac{1}{6} & \frac{1}{2} & 2 & \frac{9}{2} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

which has the solution

$$\alpha_1 = 1, \ \beta_1 = \frac{23}{12}, \beta_2 = \frac{16}{12}, \beta_3 = \frac{5}{12} .$$

Equation (2. 5) is a 3-step multivalue predictor method (Adams-Bashforth 3-step predictor). Since we wanted the local truncation error to be $0(h^4)$, it involved solving four equations in four unknowns. For a truncation error with a higher exponent, it would require solving a system of equations with more equations than unknowns which, in this case, is not possible.

Returning to the general case, suppose we now take the vector K in Equation (2. 4) to be

$$\left[\beta_o^*, 0, \ldots, 0, 1, 0, \ldots, 0\right]^T \tag{2. 6}$$

where the 1 appears in the kth position and β_o^* is some real constant. From Equations (2. 3) and (2. 2)

$$y_{n,(1)} = y_{n,(o)} + \beta_o^* \left[hf(y_{n,(o)}) - hy'_{n,(o)}\right]$$

$$= \sum_{i=1}^{k} \left[\alpha_i y_{n-i} + \beta_i hy'_{n-i} - \beta_o^* \gamma_i y_{n-i} - \beta_o^* \delta_i hy'_{n-i}\right] + \beta_o^* hf(y_{n,(o)})$$

$$= \sum_{i=1}^{k} \left[(\alpha_i - \beta_o^* \gamma_i) y_{n-i} + (\beta_i - \beta_o^* \delta_i) h y'_{n-i} \right] + \beta_o^* h f(y_{n,(o)})$$

or

$$y_{n,(1)} = \sum_{i=1}^{k} (\alpha_i^* y_{n-i} + \beta_i^* h y'_{n-i}) + \beta_o^* h f(y_{n,(o)}) \qquad (2.7)$$

where

$$\alpha_i^* = \alpha_i - \beta_o^* \gamma_i \quad \text{and} \quad \beta_i^* = \beta_i - \beta_o^* \delta_i .$$

Equations (2.4) and (2.7) then imply that

$$h y'_{n,(m+1)} = h y'_{n,(m)} - h y'_{n,(m)} + h f(y_{n,(m)})$$

$$= h f(y_{n,(m)}) \qquad (2.8)$$

and

$$y_{n,(m+1)} = y_{n,(m)} + \beta_o^* \left[h f(y_{n,(m)}) - h y'_{n,(m)} \right]$$

$$= y_{n,(1)} + h\beta_o^* \Big[f(y_{n,(m)}) + f(y_{n,(m-1)}) + \ldots + f(y_{n,(1)}) - y'_{n,(m)} - y'_{n,(m-1)} - \ldots - y'_{n,(1)} \Big]$$

$$= y_{n,(1)} + h\beta_o^* \Big[f(y_{n,(m)}) - y'_{n,(1)} \Big]$$

$$= \sum_{i=1}^{k} (\alpha_i^* y_{n-i} + \beta_i^* h y'_{n-i}) + \beta_o^* hf(y_{n,(o)}) + \beta_o^* hf(y_{n,(m)}) - \beta_o^* hy'_{n,(1)}$$

$$= \sum_{i=1}^{k} (\alpha_i^* y_{n-i} + \beta_i^* h y'_{n-i}) + \beta_o^* hf(y_{n,(m)})$$

since $f(y_{n,(o)}) = y'_{n,(1)}$ by (2.8). Thus,

$$y_{n,(m+1)} = \sum_{i=1}^{k} (\alpha_i^* y_{n-i} + \beta_i^* h y'_{n-i}) + \beta_o^* hf(y_{n,(m)}). \quad (2.9)$$

If Equations (2.8) and (2.9) are iterated to convergence, it follows that

$$y_n = \sum_{i=1}^{k} (\alpha_i^* y_{n-i} + \beta_i^* hy'_{n-i}) + \beta_o^* hf(y_n) \qquad (2.10)$$

where $hy'_{n-i} = hf(y_{n-i})$, $i = 1, 2, \ldots, k$. This is the general form of the k-step corrector multivalue method defined by (1.9). Equation (1.10) is an example of this. Derivation of (1.10) can be done using Taylor's series in the same way as (1.5) was derived. We assume a form of the method having truncation error to be $0(h^5)$ since (1.10) is of order four (this is the maximum order for the same reason given for the 3-step predictor method). For example, a form similar to (2.5) could be assumed with the term $h\beta_o y'_n$ added on. To solve for the coefficients α_1, β_i, $i = 0, 1, 2, 3$ involves solving a system of five equations in five unknowns. (Notice that the 3-step Adams-Moulton corrector method has order four while the 3-step Adams-Bashforth predictor method has order three). In Chapter 3 we will investigate methods of order r.

We now have the predictor-corrector process (2.1), (2.3), and (2.4). These are

$$y_{n,(o)} = \sum_{i=1}^{k} (\alpha_i y_{n-i} + \beta_i h y'_{n-i}) \tag{2.11}$$

and

$$y_{n,(m+1)} = \sum_{i=1}^{k} (\alpha_i^* y_{n-i} + \beta_i^* h y'_{n-i}) + \beta_o^* h f(y_{n,(m)}). \tag{2.12}$$

If (2.10) is subtracted from (2.12), then

$$y_{n,(m+1)} - y_n = \beta_o^* h \left[f(y_{n,(m)}) - f(y_n) \right] . \tag{2.13}$$

If f has a continuous derivative with respect to y, then by the Mean Value Theorem Equation (2.13) becomes

$$y_{n,(m+1)} - y_n = \beta_o^* h \frac{\partial f(\xi_n)}{\partial y} (y_{n,(m)} - y_n) \tag{2.14}$$

where $\xi_n \in (y_{n,(m)}, y_n)$. Thus, if h is chosen sufficiently small so that $\left| h \beta_o^* \frac{\partial f}{\partial y} \right| < 1$ within the region of interest and $\left| y_{n,(m+1)} - y_n \right| < \left| y_{n,(m)} - y_n \right|$, then the iteration (2.12) will converge to the solution of (2.10) (since by (2.14) $\left| y_{n,(m+1)} - y_n \right| \leq \left| \beta_o^* h \dfrac{\partial f(\xi_n)}{\partial y} \right| \left| y_{n,(m)} - y_n \right|$).

The predictor and corrector formulas need not be of the same order. If the predictor has order q and the corrector r, then from (2.11)

$$y(t_n) = \sum_{i=1}^{k} \left[\alpha_i y(t_{n-i}) + h \beta_i y'(t_{n-i}) \right] + 0(h^{q+1})$$

$$= y_{n,(o)} + 0(h^{q+1}). \quad \text{(Predictor formula)} \tag{2.15}$$

$$y(t_n) = \sum_{i=1}^{k} \left[\alpha_i^* y(t_{n-i}) + \beta_i^* h y'(t_{n-i}) \right] + \beta_o^* h f(y(t_n)) + 0(h^{r+1})$$

$$= \sum_{i=1}^{k} \left[\alpha_i^* y(t_{n-i}) + \beta_i^* h y'(t_{n-i}) \right] + \beta_o^* h f(y_{n,(o)}) + \beta_o^* h f(y(t_n))$$

$$- \beta_o^* h f(y_{n,(o)}) + 0(h^{r+1})$$

$$= y_{n,(1)} + h\beta_o^* \left[f(y(t_n)) - f(y_{n,(o)}) \right] + 0(h^{r+1}) \tag{2.16}$$

by (2.7). Using the Mean Value Theorem and (2.15), (2.16) becomes

$$y(t_n) = y_{n,(1)} + h\beta_o^* \frac{\partial f(\tilde{\xi}_n)}{\partial y}\left[y(t_n) - y_{n,(o)}\right] + 0(h^{r+1})$$

$$= y_{n,(1)} + h\beta_o^* \frac{\partial f(\tilde{\xi}_n)}{\partial y}\left[y_{n,(o)} + 0(h^{q+1}) - y_{n,(o)}\right] + 0(h^{r+1})$$

$$= y_{n,(1)} + 0(h^{q+2}) + 0(h^{r+1}) \quad \text{(first application of corrector)}$$

where $\tilde{\xi}_n \epsilon (y(t_n), y_{n,(o)})$. If we continue this in like fashion until the mth application of the corrector is reached, we get

$$y(t_n) = y_{n,(m)} + o(h^{q+m+1}) + 0(h^{r+1}).$$

Thus, each additional corrector application will increase the order of solution by one until convergence is reached. However, in practice we do not wish to correct many times, because each additional corrector step requires an additional function evaluation for the derivative. Usually q is taken to be r−1 or r and about two corrector steps are used.

CHAPTER III

GENERAL MULTIVALUE METHODS

In the previous chapter we examined two particular multivalue methods, a predictor and a corrector, that are very effective for integrating many differential equations. In this chapter we will examine general k-step methods of the form

$$\sum_{i=0}^{k} (\alpha_i y_{n-i} + h\beta_i f_{n-i}) = 0 \qquad (3.1)$$

where $f_j = f(y_j, t_j)$ and discuss the subject of stability.

Define

$$L_h(y(t)) = \sum_{i=0}^{k} \left[\alpha_i y(t-ih) + h\beta_i y'(t-ih)\right] . \qquad (3.2)$$

The order of the operator L_h will be defined as follows (see Gear [1, p. 118]):

Definition 3.1

The order of the operator L_h is the largest integer r such that if y(t) has a continuous (r+1)th derivative, then

$$L_h(y(t)) = 0(h^{r+1}).$$

In Chapter II the α's and β's of a multivalue method of order r were determined by the method of undetermined coefficients. If we assume a continuous (r+2)th derivative for y, then we can substitute the Taylor's series for y and y' in (3.2) with $0(h^{r+2})$ remainders to get

$$L_h(y(t)) = \sum_{i=0}^{k} \left[\alpha_i y(t-ih) + h\beta_i y'(t-ih)\right]$$

$$= \sum_{i=0}^{k} \Big[\alpha_i (y(t) - ihy'(t) + \frac{(ih)^2}{2!} y''(t) + \ldots + \frac{(-1)^{r+1}(ih)^{r+1}}{(r+1)!} y^{(r+1)}(t))$$

$$+ h\beta_i (y'(t) - ihy''(t) + \frac{(ih)^2}{2!} y^{(3)}(t) + \ldots + \frac{(-1)^{r-1}(ih)^{r-1}}{(r-1)!} y^{(r)}(t)$$

$$+ \frac{(-1)^r (ih)^r}{r!} y^{(r+1)}(t)) + 0(h^{r+2})\Big]$$

$$= \sum_{i=0}^{k} \Big[\alpha_1 h^0 y^{(t)} + (-i\alpha_i + \beta_i) h y'(t) + \left(\frac{i^2\alpha_i}{2!} - i\beta_i\right) h^2 y''(t)$$

$$+ \ldots + \left(\frac{(-i)^{r+1}\alpha_i}{(r+1)!} + \frac{(-i)^r \beta_i}{r!}\right) h^{r+1} y^{(r+1)}(t)\Big] + 0(h^{r+2})$$

$$= \left(\sum_{i=0}^{k} \alpha_1\right) h^0 y^{(0)}(t) + \left(\sum_{i=0}^{k} \left((-i)\alpha_i + \beta_i\right)\right) h y^{(1)}(t)$$

$$+ \left(\sum_{i=0}^{k} \left(\frac{(-i)^2\alpha_i}{2!} + \frac{(-i)\beta_i}{1!}\right)\right) h^2 y^{(2)}(t)$$

$$+ \ldots + \left(\sum_{i=0}^{k} \left(\frac{(-i)^{r+1}\alpha_i}{(r+1)!} + \frac{(-1)^r \beta_i}{r!}\right)\right) h^{r+1} y^{(r+1)}(t) + 0(h^{r+2})$$

$$= \left(\sum_{i=0}^{k} \alpha_i\right) y(t) + \sum_{q=1}^{r+1} \sum_{i=0}^{k} \left(\frac{(-i)^q\alpha_i}{q!} + \frac{(-i)^{q-1}\beta_i}{(q-1)!}\right) h^q y^{(q)}(t) + 0(h^{r+2})$$

$$= \sum_{q=0}^{r+1} C_q h^q y^{(q)}(t) + 0(h^{r+2}).$$

Therefore,

$$L_h(y(t)) = \sum_{q=0}^{r+1} C_q h^q y^{(q)}(t) + 0(h^{r+2}) \tag{3.3}$$

where

$$C_q = \begin{cases} \sum_{i=0}^{k} \alpha_i, \; q = 0 \\ \\ \sum_{i=0}^{k} \left[\frac{(-i)^q}{q!}\alpha_i + \frac{(-i)^{q-1}}{(q-1)!}\beta_i \right], \; q > 0. \end{cases} \tag{3.4}$$

The linear equations $C_q = 0$, $q \leq r$ yield the values of the α's and β's, hence determine the rth order multivalue method. C_{r+1} is the truncation error coefficient of L_h and depends only on the coefficients of the multivalue method, not on y or the point of expansion t. So (3,3) can be written as

$$L_h(y(t)) = \sum_{i=0}^{k} \left[\alpha_i y(t-ih) + h\beta_i y'(t-ih)\right]$$

$$= C_{r+1} h^{r+1} y^{(r+1)}(t) + 0(h^{r+2}). \tag{3.5}$$

Let

$$e_n = y_n - y(t_n) \tag{3.6}$$

which signifies the amount of truncation error introduced at each step in using (3.1) to solve first order equations on $[0, b]$. To determine e_n, we assume f has a continuous second derivative on $[0, b]$ and prove the following theorem:

Theorem 3.1

Let $\delta(t)$ be some function of t whose first derivative is

$$\delta'(t) = g(t)\,\delta(t) + \frac{C_{r+1}\, y^{(r+1)}(t)}{\sum_{j=0}^{k} \beta_j},$$

where $\delta(0) = e_o/h^r$, $g(t) = f_y(y(t))$, and C_{r+1} is defined as in (3.4). Then the error e_n for a convergent multivalue method for first order equations is

$$e_n = h^r\,\delta(t_n) + 0(h^{r+1})$$

where $\delta(t)$ satisfies the above differential equation.

Proof: First, subtract (3.5) from (3.1) to get

$$\sum_{i=0}^{k}\Big[(y_{n-i} - y(t_n - ih))\alpha_i + h\beta_i(f(y_{n-i}) - f(y(t_n - ih))\Big]$$

$$= -C_{r+1}h^{r+1}y^{(r+1)}(t_n) + 0(h^{r+2}). \quad (3.7)$$

Then, by the Mean Value Theorem

$$f(y_{n-i}) - f(y(t_{n-i})) = e_{n-i}f_y(\xi_{n-i}),\ \xi_{n-i}\epsilon(y_{n-i}, y(t_{n-i})) \qquad (3.8)$$

where $f_y(\xi_{n-i}) = \dfrac{\partial f(\xi_{n-i})}{\partial y}$. Therefore, using (3.6) and (3.8), (3.7) becomes

$$\sum_{i=0}^{k}\alpha_i e_{n-i} + h\beta_i f_y(\xi_{n-i})e_{n-i} + C_{r+1}h^{r+1}y^{(r+1)}(t_n) = 0(h^{r+2})$$

or

$$\sum_{i=0}^{k}\left[\alpha_i e_{n-i} + h\beta_i f_y(\xi_{n-i})e_{n-i} + \frac{C_{r+1}\beta_i h^{r+1} y^{(r+1)}(t_n)}{\sum_{j=0}^{k}\beta_j}\right] = 0(h^{r+2}). \quad (3.9)$$

Expanding $y^{(r+1)}(t_{n-1})$ in a Taylor's series about t_n and solving for $y^{(r+1)}(t_n)$ yields

$$y^{(r+1)}(t_n) = y^{(r+1)}(t_{n-i}) + 0(h). \qquad (3.10)$$

If $f(y_{n-i})$ is expanded in a Taylor's series about $y(t_{n-i})$ then

$$f(y_{n-i}) = f(y(t_{n-i})) + e_{n-i} f_y(y(t_{n-i})) + \frac{e_{n-i}^2}{2} f_{yy}(\xi_{n-i}^*) \qquad (3.11)$$

where

$$f_{yy}(\xi_{n-i}^*) = \frac{\partial^2 f(\xi_{n-i}^*)}{\partial y^2}, \quad \xi_{n-i}^* \in (y_{n-i}, y(t_{n-i})).$$

Subtracting $f(y(t_{n-i}))$ from both sides of (3.11) yields

$$f(y_{n-i}) - f(y(t_{n-i})) = e_{n-i} f_y(y(t_{n-i})) + e_{n-i}^2 f_{yy}(\xi_{n-i}^*). \quad (3.12)$$

Since the left sides of Equations (3.8) and (3.12) are equal, it follows that

$$e_{n-i} f_y(\xi_{n-i}) = e_{n-i} f_y(y(t_{n-i})) + e_{n-i}^2 f_{yy}(\xi_{n-i}^*)$$

or

$$f_y(\xi_{n-i}) = f_y(y(t_{n-i})) + e_{n-i} f_{yy}(\xi_{n-i}^*). \quad (3.13)$$

Set

$$e_n = h^r \delta_n \quad (3.14)$$

where δ_n is some function of t and is to be determined. (It will be seen later that δ_n is a continuous function of t on [0, b]. Assume for now that δ_n is continuous on [0, b]). Therefore, by using Equation (3.14), (3.13) becomes

$$f_y(\xi_{n-i}) = f_y(y(t_{n-i})) + 0(h^r). \tag{3.15}$$

Substitute (3.10), (3.14), and (3.15) into (3.9) to get

$$\sum_{i=0}^{k}\left[\alpha_i\delta_{n-i} + h\beta_i\left(f_y(y(t_{n-i}))\delta_{n-i} + \frac{C_{r+1}y^{(r+1)}(t_{n-i})}{\sum_{j=0}^{k}\beta_j} + 0(h)\right)\right] = 0. \tag{3.16}$$

This is the solution, by (3.1), of the differential equation

$$\delta'(t) = g(t)\delta(t) + \frac{C_{r+1}y^{(r+1)}(t)}{\sum_{j=0}^{k}\beta_j} \tag{3.17}$$

where $g(t) = f_y(y(t))$. (Note that if $\delta'(t)$ is defined on $[0, b]$ as in (3.17), then $\delta(t)$ is continuous on $[0, b]$). It follows from (3,14) that (3.17) has the initial condition $\delta(0) = e_o/h^r$. Now, $\left|\frac{\partial\delta'(t)}{\partial\delta(t)}\right| = |g(t)|$ which is bounded on $[0, b]$ since $g(t) = f_y(y(t))$ is (it has been assumed that f satisfies a Lipschitz condition in y). Thus, $\delta'(t)$ satisfies the Lipschitz condition in δ which implies that (3.17) is well-posed (see Theorem 1.2). Assume that (3.1) is stable. Then for sufficiently small h, (3.16) approximates the solution of (3.17) since (3.17) differs from the numerical solution (3.16) by $0(h)$ at most. Thus, (3.14) becomes

$$e_n = h^r(\delta_n + 0(h))$$

$$= h^r \delta_n + 0(h^{r+1}).$$

Therefore, for a convergent multivalue method for first order equations $e_n = h^r \delta(t_n) + 0(h^{r+1})$ where $\delta(t)$ satisfies (3.17) with $\delta(0) = e_o/h^r$. Q. E. D.

A natural normalization [see Equations (3.16) and (3.17)] of a multivalue method is to make

$$\sum_{i=0}^{k} \beta_i = 1. \tag{3.18}$$

It will be assumed that this has been done when we discuss the error coefficient C_{r+1}.

It is desirable to have some kind of condition on the multivalue method so that it will have order r. To get this condition, we first associate with the k-step multivalue method defined by Equation (3.1) the polynomials

$$\rho(\xi) = \sum_{i=0}^{k} \alpha_i \xi^{k-i} \tag{3.19}$$

$$\sigma(\xi) = \sum_{i=0}^{k} \beta_i \xi^{k-i} \tag{3.20}$$

where the maximum degree of ρ and σ is the step number (which is k) of the multivalue method. A condition follows from

Theorem 3. 2.

A necessary and sufficient condition that a multivalue method have order r is that

$$\rho(1+z) + \log(1+z)\sigma(1+z) = C_{r+1} z^{r+1} + 0(z^{r+2})$$

where z is a complex number.

Proof: For the necessary condition, consider the function $y(t) = e^{\lambda t}$ where λ is a complex number. Then from (3. 2), (3.19), and (3. 20)

$$L_h(y(t)) = \sum_{i=0}^{k} (\alpha_i + \lambda h \ \beta_i) e^{\lambda(t-ih)}$$

$$= \sum_{i=0}^{k} e^{\lambda(t-hk)} (\alpha_i + h\lambda\beta_i)(e^{h\lambda})^{k-i}$$

$$= e^{\lambda(t-hk)} \sum_{i=0}^{k} (\alpha_i + h\lambda\beta_i)(e^{h\lambda})^{k-i}$$

$$= e^{\lambda(t-hk)} \left[\rho(e^{h\lambda}) + h\lambda\sigma(e^{h\lambda}) \right] . \qquad (3.21)$$

Since $e^{hk} = 1 + 0(h)$, then by Equation (3.5)

$$L_h(y(t)) = C_{r+1} h^{r+1} y^{(r+1)}(t) + 0(h^{r+2})$$

$$= C_{r+1} (h\lambda)^{r+1} e^{\lambda t} + 0(h^{r+2})$$

$$= C_{r+1} (h\lambda)^{r+1} e^{\lambda t} - C_{r+1} (h\lambda)^{r+1} e^{\lambda(t-hk)}$$

$$+ C_{r+1} (h\lambda)^{r+1} e^{\lambda(t-hk)} + 0(h^{r+2})$$

$$= C_{r+1}(h\lambda)^{r+1}\left[e^{\lambda t} - e^{\lambda t} \cdot e^{-\lambda hk}\right] + C_{r+1}(h\lambda)^{r+1} e^{\lambda(t-hk)} + 0(h^{r+2})$$

$$= e^{\lambda t} C_{r+1}(h\lambda)^{r+1}\left[1 - e^{-\lambda hk}\right] + C_{r+1}(h\lambda)^{r+1} e^{\lambda(t-hk)} + 0(h^{r+2})$$

$$= e^{\lambda t} C_{r+1}(h\lambda)^{r+1}\left[1-(1-0(h))\right] + C_{r+1}(h\lambda)^{r+1} e^{\lambda(t-hk)} + 0(h^{r+2})$$

$$= C_{r+1}(h\lambda)^{r+1} e^{\lambda(t-hk)} + 0(h^{r+2}). \qquad (3.22)$$

Therefore, from (3.21) and (3.22)

$$\rho(e^{h\lambda}) + h\lambda\sigma(e^{h\lambda}) = C_{r+1}(h\lambda)^{r+1} + 0(h^{r+2}). \qquad (3.23)$$

Let $h\lambda = \log(1+z)$ where z is a complex number. If we consider the power series expansion of $\log(1+z)$ where $|z| < 1$, then $h\lambda = \log(1+z) = z + 0(z^2)$. Then (3.23) becomes

$$\rho(1+z) + \log(1+z)\sigma(1+z) = C_{r+1}(z+0(z^2))^{r+1} + 0(h^{r+2})$$

$$= C_{r+1}\left[z^{r+1} + \frac{(r+1)!}{r!\,1!} z^r(0(z^2))\right.$$

$$\left. + \ldots + (0(z^2))^{r+1}\right] + 0\left(\left(\frac{z+0(z^2)}{\lambda}\right)^{r+2}\right)$$

$$= C_{r+1} z^{r+1} + z^{r+2}\left[C_{r+1}\frac{(r+1)!}{r!\,1!}k_1 + \ldots + 0(z^r)\right]$$

$$+ 0(z^{r+2})$$

$$= C_{r+1} z^{r+1} + 0(z^{r+2})$$

where k_1 is some constant. Therefore,

$$\rho(1+z) + \log(1+z)\sigma(1+z) = C_{r+1} z^{r+1} + 0(z^{r+2}) \qquad (3.24)$$

which shows the necessary condition of the theorem. For the sufficiency part of the theorem, it follows from Equation (3.3) and Definition 3.1 that

$$L_h(e^{\lambda t}) = \sum_{q=0}^{\infty} C_q (h\lambda)^q e^{\lambda t}$$

$$= 0(h^{r+1}).$$

This implies that $C_o = C_1 = \ldots = C_r = 0$. Thus, (3.24) is also a sufficient condition that a multivalue method have order r. Q.E.D. Expanding (3.24) in a power series about z, it follows that

$$\rho(1) + z\rho'(1) + 0(z^2) + [z + 0(z^2)]\,[\sigma(1) + 0(z)]$$

$$= \rho(1) + z[\rho'(1) + \sigma(1)] + 0(z^2)$$

$$= C_{r+1} z^{r+1} + 0(z^{r+2}).$$

Therefore,

$$\rho(1) + z[\rho'(1) + \sigma(1)] + 0(z^2) = C_{r+1} z^{r+1} + 0(z^{r+2})$$

from which it is seen that for order $r \geq 0$

$$\rho(1) = 0 \qquad (3.25)$$

and for order $r \geq 1$

$$\rho'(1) + \sigma(1) = 0 \qquad (3.26)$$

where $\sigma(1) = 1$ [see Equations (3.20) and (3.18)].

Theorem 3.2 tends to be quite useful as is seen in the following theorem:

Theorem 3.3

If the polynomial $\sigma(1+z)$ of degree $j \leq k$ is given in Equation (3.24), a polynomial $\rho(1+z)$ of degree k can be found such that the multivalue method has order $r \geq k$.

Proof: The polynomial σ is given. Let [see Equation (3.20)]

$$\sigma(1+z) = \sum_{i=0}^{j} \beta_i (1+z)^{j-i}$$

$$= \sum_{i=0}^{j} \sum_{\ell=0}^{j-i} \beta_i \binom{j-i}{\ell} z^{\ell}$$

$$= \sum_{i=0}^{j} \sum_{\ell=0}^{j-i} \beta_{\ell} \binom{j-\ell}{i} z^{i}$$

$$= \sum_{i=0}^{j} b_i z^i \qquad (3.27)$$

where

$$b_i = \sum_{\ell=0}^{j-i} \beta_\ell \binom{j-\ell}{i}, \quad j \leq k \tag{3.28}$$

and $\binom{n}{m} = \frac{n!}{m!\,(n-m)!}$ (note that $b_i = 0$ for $i > j$). Since σ is known, the β_ℓ's are known, hence the b_i's. Let [see Equation (3.19)]

$$\rho(1+z) = \sum_{i=0}^{k} \alpha_i (1+z)^{k-i}$$

$$= \sum_{i=0}^{k} a_i z^i \tag{3.29}$$

where

$$a_i = \sum_{\ell=0}^{k-i} \alpha_\ell \binom{k-\ell}{i} \tag{3.30}$$

and $a_i = 0$ for $i > k$. We want to solve for these a_i, $i = 0, 1, \ldots, k$ so that the multivalue method has order $r \geq k$. From Equation (3.24) it follows that

$$\rho(1+z) + \log(1+z)\sigma(1+z) = \sum_{i=0}^{k} a_i z^i + \left(z - \frac{z^2}{2} + \frac{z^3}{3} - \cdots\right) \sum_{i=0}^{j} b_i z^i$$

$$= a_o + \sum_{i=1}^{k} \sum_{\ell=0}^{i-1} \left(a_i + (-1)^{i-\ell+1} \frac{b_\ell}{i-\ell} \right) z^i$$

$$+ \sum_{i=k+1}^{\infty} \sum_{\ell=0}^{i-1} (-1)^{i-\ell+1} \frac{b_\ell}{i-\ell} \qquad (3.31)$$

where $b_\ell = 0$ for $\ell > j$. Set

$$a_o = 0$$

$$a_i = \sum_{\ell=0}^{i-1} (-1)^{i+\ell} \frac{b_\ell}{i-\ell}, \quad i = 1, 2, \ldots, k. \qquad (3.32)$$

By doing this, the term $a_o + \sum_{i=1}^{k} \sum_{\ell=0}^{i-1} (a_i + (-1)^{\ell+1} \frac{b_\ell}{i-\ell}) z^i$

in Equation (3.31) becomes zero. Therefore, Equation (3.31) becomes

$$\rho(1+z) = \log(1+z)\sigma(1+z) = \sum_{i=k+1}^{\infty} \sum_{\ell=0}^{i-1} (-1)^{i-\ell+1} \frac{b_\ell}{i-\ell}$$

$$= \sum_{i=k+1}^{\infty} c_i z^i \tag{3.33}$$

where

$$c_i = \sum_{\ell=0}^{i-1} (-1)^{i-\ell+1} \frac{b_\ell}{i-\ell}, \quad i = k+1, \ldots . \tag{3.34}$$

The c_i's determine the order of the multivalue method. The first c_i, $i \geq k+1$ that is not zero implies the method will be of order $r = i-1$. Hence, if the a_i, $i = 0, 1, \ldots, k$ in Equation (3.29) are picked according to (3.32), then the multivalue method will have order $r \geq k$. (Note that the α_i's, $i = 0, 1, \ldots, k$ can be found so the multivalue method will have order $r > k$ by setting Equation (3.30) to (3.32) and solving for the α's). Q. E. D.

To illustrate Theorem 3.3 consider the following example:

Example 3.1

Let $\sigma(\xi) = \frac{3}{2}\xi - \frac{1}{2}$ and $k = 2$. Therefore,

$$\sigma(1+z) = \frac{3}{2}(1+z) - \frac{1}{2}$$

which implies that $\beta_o = \frac{3}{2}$, $\beta_1 = -\frac{1}{2}$, $\beta_2 = 0$, and $j = 1$. Let [see Equation (3. 29)]

$$\rho(1+z) = \sum_{i=0}^{2} a_i z^i$$

where the a_i are to be determined so that the multivalue method will have order $r \geq 2$. The $a_i = 0$ for $i > 2$ since $k = 2$. Therefore, by (3.32) and (3. 28) it follows that $a_o = 0$ and

$$a_1 = -b_o$$

$$= -\sum_{\ell=0}^{1} \beta_\ell \binom{1-\ell}{0}$$

$$= -\beta_o - \beta_1$$

$$= -1$$

and

$$a_2 = \sum_{\ell=0}^{1} (-1)^{2-\ell} \frac{b_\ell}{2-\ell}$$

$$= \frac{b_o}{2} - b_1$$

$$= \frac{1}{2} - \beta_o$$

$$= -1.$$

Therefore, $a_o = 0$, $a_1 = -1$, $a_2 = -1$, $b_o = 1$, and $b_1 = \frac{3}{2}$.

Thus, it follows from (3.29) that

$$\rho(1+z) = -z - z^2$$

$$= -(1+z)^2 + (1+z). \qquad (3.35)$$

Hence, in this case where k = 2 [see Equation (3.29)] Equation (3.35) implies that

$$\alpha_o = -1, \ \alpha_1 = 1, \ \alpha_2 = 0.$$

So it follows from Equation (3.19) that

$$\rho(\xi) = -\xi^2 - \xi .$$

By the way the α_i and β_i, i = 0, 1, 2 were picked, it is seen from Equation (3.1) that the multivalue method is

$$-y_n + y_{n-1} + \frac{3}{2} hy'_{n-1} - \frac{h}{2} y'_{n-2} = 0. \qquad (3.37)$$

Theorem 3.3 guarantees us that it has order $r \geq 2$. To determine r, we use (3.34). Therefore, for i = 3

$$c_3 = \sum_{\ell=0}^{2} (-1)^{4-\ell} \frac{b_\ell}{3-\ell}$$

$$= \frac{b_o}{3} - \frac{b_1}{2} + b_2$$

$$= \frac{1}{3} - \frac{3}{4} + 0$$

$$= -\frac{5}{12} .$$

(Recall that $b_i = 0$ for $i > j$.) Since $c_3 \neq 0$, it implies that the order r of Equation (3.37) is r = 2. Equation (3.37) is the second order 2-step Adams-Bashforth predictor multivalue method.

(An easier way of picking $\rho(\xi)$ where σ is given can be done by setting $r = k$ in Equation (3.24) to get

$$\rho(1+z) = -\log(1+z)\sigma(1+z) + C_{i+1} z^{k+1} + 0(z^{k+2}).$$

If $v(z)$ is set to be the terms in z^j $(0 \le j \le k)$ in the expansion of $-\log(1+z)\sigma(1+z)$, then $\rho(\xi)$ is given by $\rho(\xi) = v(\xi - 1)$.)

Suppose this time that ρ is given. Then Theorem 3.2 can be used to show that a polynomial σ of degree k can be found so that the multivalue method will have order $r \geq k+1$. To see this, we will prove the following theorem:

Theorem 3.4

If the polynomial $\rho(1+z)$ of degree $j \leq k$ is given in Equation (3.24), a polynomial $\sigma(1+z)$ of degree k can be found such that the multivalue method has order $r \geq k+1$.

Proof: The same thing will be done here that was done in the proof of Theorem 3.3 except this time $\rho(1+z)$ is given and say is of degree $j \leq k$ and a polynomial $\sigma(1+z)$ of degree k is to be found. Let

$$\rho(1+z) = \sum_{i=0}^{j} a_i z^i \tag{3.38}$$

where

$$a_i = \sum_{\ell=0}^{j-i} \alpha_\ell \binom{j-\ell}{i}, \quad j \leq k \tag{3.39}$$

[see Equations (3. 29) and (3. 30)] and $a_i = 0$ for $i > j$. Since ρ is known, the α_ℓ's are known, hence the a_i's. Let

$$\sigma(1+z) = \sum_{i=0}^{k} b_i z^i \tag{3.40}$$

where

$$b_i = \sum_{\ell=0}^{k-i} \beta_\ell \binom{k-\ell}{i} \tag{3.41}$$

[see Equations (3. 27) and (3. 28)] and $b_i = 0$ for $i > k$. Thus, from Equation (3. 24)

$$\rho(1+z) + \log(1+z)\sigma(1+z) = \sum_{i=1}^{j} a_i z^i + \left(z - \frac{z^2}{2} + \frac{z^3}{3} - \cdots\right) \sum_{i=1}^{k} b_i z^i$$

$$= a_o + \sum_{i=1}^{j} \sum_{\ell=0}^{i-1} \left(a_i + (-1)^{i-\ell+1} \frac{b_\ell}{i-\ell} \right) z^i$$

$$+ \sum_{i=j+1}^{\infty} \sum_{\ell=0}^{i-1} (-1)^{i-\ell+1} \frac{b_\ell}{i-\ell} z^i \tag{3.42}$$

where $b_\ell = 0$ for $\ell > k$. A multivalue method having order $r \geq 0$ implies that $\rho(1) = 0$ [see Equation (3.25)]. Hence, $a_o = 0$. The a_i, $i = 1, 2, \ldots, j$ are known. Therefore, set

$$\sum_{\ell=0}^{i-1} (-1)^{i-\ell+1} \frac{b_\ell}{i-\ell} = -a_i, \quad i = 1, 2, \ldots, j \tag{3.43}$$

in Equation (3.42) and solve for the b_i. That is,

$$a_o = 0$$

$$b_o = -a_1$$

$$b_1 = -a_2 + \frac{b_o}{2} = -a_2 - \frac{a_1}{2}$$

$$b_2 = -a_3 = \frac{b_1}{2} - \frac{b_o}{3} = -a_3 - \frac{a_2}{2} + \frac{a_1}{12}$$

$$b_3 = -a_4 + \frac{b_2}{2} - \frac{b_1}{3} + \frac{b_o}{4} = -a_4 - \frac{a_3}{2} + \frac{a_2}{12} - \frac{a_1}{24}$$

$$
\begin{aligned}
&\vdots \\
&\vdots \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.44) \\
&\vdots \\
b_{j-1} &= -a_j + \frac{b_{j-2}}{2} - \frac{b_{j-3}}{3} + \ldots + (-1)^j \frac{b_o}{j}
\end{aligned}
$$

where the b_{j-2}, b_{j-3}, . . . , b_o can be solved in terms of the a_i, $0 \leq i \leq j$. Now, $a_i = 0$ for $i > j$. Therefore,

$$
\begin{aligned}
b_j &= \frac{b_{j-1}}{2} - \frac{b_{j-2}}{3} + \ldots + (-1)^{j+1} \frac{b_o}{j+1} \\
&\vdots \\
&\vdots \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.45) \\
&\vdots \\
b_k &= \frac{h_{k-1}}{2} - \frac{h_{k-2}}{3} + \ldots + (-1)^{k+1} \frac{b_o}{k+1}
\end{aligned}
$$

where the b_{i-1}, b_{i-2}, . . . , b_o, $j \leq i \leq k$ can be solved in terms of the a_i, $0 \leq i \leq j$. If the b_i, $i = 0, 1, \ldots, k$ are picked in this fashion, then Equation (3.42) becomes

$$\rho(1+z) + \log(1+z)\sigma(1+z) = \sum_{i=k+2}^{\infty} \sum_{\ell=0}^{i-1} (-1)^{i-\ell+1} \frac{b_\ell}{i-\ell} z^i$$

$$= \sum_{i=k+2}^{\infty} h_i z^i \tag{3.46}$$

where

$$h_i = \sum_{\ell=0}^{i-1} (-1)^{i-\ell+1} \frac{b_\ell}{i-\ell}, \quad i = k+2, \ldots . \tag{3.47}$$

The first h_i, $i \geq k+2$ that is nonzero implies that the method will be of order $r = i-1$ (note that

$$h_{k+2} = -\frac{b_k}{2} + \frac{b_{k-1}}{3} - \frac{h_{k-2}}{4} + \ldots + (-1)^{k+3} \frac{b_o}{k+2}$$

which may or may not be zero). Hence, it follows from (3.46) that the multivalue method will have order $r \geq k+1$. Q. E. D.

To illustrate Theorem 3.4, consider the following example:

Example 3.2

Let $\rho(\xi) = -\xi^2 + \xi$ and $k = 2$. Then

$$\rho(1+z) = -(1+z)^2 + (1+z)$$

which implies that $\alpha_o = -1$, $\alpha_1 = 1$, $\alpha_2 = 0$ and $j = 2$.

Let

$$\sigma(1+z) = \sum_{i=0}^{2} b_i z^i$$

where the b_i are to be determined so that the multivalue method will have order $r \geq 3$. To determine the b_i, Equation (3.39) must first be used to determine the a_i, then (3.44) and (3.45) can be used to find the b_i, $i = 0, 1, 2$ (recall that $b_i = 0$ for $i > k$ and $a_i = 0$ for $i > j$). Hence, by Equation (3.39)

$$a_o = \sum_{\ell=0}^{2} \alpha_\ell \binom{2-\ell}{0}$$

$$= \alpha_o + \alpha_1 + \alpha_2$$

$$= 0$$

and

$$a_1 = \sum_{\ell=0}^{1} \alpha_\ell \binom{2-\ell}{1}$$

$$= 2\alpha_o + \alpha_1$$

$$= -1$$

and

$$a_2 = \alpha_o$$

$$= 2\alpha_o + \alpha_1$$

$$= -1.$$

Therefore, $a_o = 0$, $a_1 = -1$, and $a_2 = -1$. By (3.44) and (3.45)

$$b_o = -a_1$$

$$= 1$$

and

$$b_1 = -a_2 - \frac{a_1}{2}$$

$$= \frac{3}{2}$$

and

$$b_2 = \frac{b_1}{2} - \frac{b_o}{3}$$

$$= \frac{5}{12}.$$

Thus, Equation (3.40) becomes

$$\sigma(1+z) = 1 + \frac{3}{2} z + \frac{5}{12} z^2$$

$$= \frac{5}{12}(1+z)^2 + \frac{2}{3}(1+z) - \frac{1}{12}. \qquad (3.48)$$

Recall that $\sigma(1+z) = \sum_{i=0}^{k} b_i z^i = \sum_{i=0}^{k} \beta_i (1+z)^{k-i}$. Therefore,

in this case where k = 2, Equation (3.48) implies that $\beta_o = \frac{5}{12}$, $\beta_1 = \frac{2}{3}$, and $\beta_2 = -\frac{1}{12}$. Hence, it follows from Equation (3.20) that

$$\sigma(\xi) = \frac{5}{12}\,\xi^2 + \frac{2}{3}\,\xi - \frac{1}{12}.$$

It follows from Equation (3.1) that the multivalue method is

$$-y_n + y_{n-1} + \frac{5}{12}\,hy'_n + \frac{2}{3}\,hy'_{n-1} - \frac{1}{12}\,hy_{n-2} = 0. \quad (3.49)$$

To determine the order of (3.48), Equation (3.47) is used. For i = 4

$$h_4 = \sum_{\ell=0}^{3} (-1)^{5-\ell}\,\frac{b_\ell}{4-\ell}$$

$$= -\frac{b_o}{4} + \frac{b_1}{3} - \frac{b_2}{2} + \frac{b_3}{1}$$

$$= -\frac{1}{4} + \frac{1}{2} - \frac{5}{24} + 0$$

$$= \frac{1}{24}\ .$$

So $h_4 \neq 0$ which implies that the order of Equation (3.49) is r = 3. Equation (3.49) is the third order 2-step Adams-Moulton corrector method.

Theorems 3.3 and 3.4 guarantee us that a k-step multivalue method of order $r \geq k$ can be found. The question now is how large can r be? As an example, note that there are 2k+2 unknowns in Equation (3.1). To solve for these unknowns, (3.4) was derived. For q = 2k the following system of equations is found:

$$\begin{bmatrix} 1 & & & 1 & 0 & & & 0 \\ 0 & -1 & \cdots & -k & 1 & & & 1 \\ 0 & \frac{1^2}{2!} & \cdots & \frac{k^2}{2!} & 0 & -1 & \cdots & -k \\ 0 & -\frac{1^3}{3!} & \cdots & -\frac{k^3}{3!} & 0 & \frac{1^2}{2!} & \cdots & \frac{k^2}{2!} \\ 0 & \frac{1^4}{4!} & \cdots & \frac{k^4}{4!} & 0 & -\frac{1^3}{3!} & \cdots & -\frac{k^3}{3!} \\ \cdot & & & & & & & \cdot \\ \cdot & & & \cdot & & \cdot & \cdot & \cdot \\ \cdot & & & & & & & \cdot \\ 0 & \frac{(-1)^{2k}}{(2k)!} & \cdots & \frac{(-k)^{2k}}{(2k)!} & 0 & \frac{(-1)^{2k-1}}{(2k-1)!} & \cdots & \frac{(-k)^{2k-1}}{(2k-1)!} \end{bmatrix} \begin{bmatrix} \alpha_o \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \cdot \\ \cdot \\ \alpha_k \\ \beta_o \\ \beta_1 \\ \cdot \\ \cdot \\ \cdot \\ \beta_k \end{bmatrix} = \begin{bmatrix} C_o \\ C_1 \\ C_2 \\ C_3 \\ \cdot \\ \cdot \\ C_k \\ \cdot \\ \cdot \\ \cdot \\ C_{2k} \end{bmatrix} . \tag{3.50}$$

This is a system of 2k+1 equations in 2k+2 unknowns. Hence, for q = 2k the α_i and β_i, i = 0, 1, . . . , k can be found so that $C_o = C_1 = \ldots = C_{2k} = 0$ [see (3.4)] which implies that the multivalue method will have order $r \geq 2k$. If the normalization $\sum_{i=0}^{k} \beta_i = 1$ defined by (3.18) is used, then we will have a system of 2k+2 nonhomogenous equations in 2k+2 unknowns. If the system is nonsingular, there exists a unique solution for the α_i and β_i, $i = 0, 1, \ldots, k$ such that $C_o = C_1 = \ldots = C_{2k} = 0$. So again the multivalue method will have order $r \geq 2k$. It will be seen later that k-step multivalue methods having order $r > k+1$ where k is odd and order $r > k+2$ where k is even are unstable. Therefore, it is unnecessary to find multivalue methods having order $r > k+2$.

The concept of stability of a k-step multivalue method is introduced as follows. Suppose that the multivalue method (3.1) is applied to the differential equation $y' = \lambda y$. Then

$$\sum_{i=0}^{k} (\alpha_i + h\lambda\beta_i) y_{n-i} = 0. \tag{3.51}$$

A solution to (3.51) of the form $y_n = p\,\xi^n$, p a constant, can be found if ξ is a root of the equation

$$\sum_{i=0}^{k} (\alpha_i + h\lambda\beta_i)\xi^{k-i} = \rho(\xi) + h\lambda\sigma(\xi) = 0. \tag{3.52}$$

Since the solution of $y' = \lambda y$ is $y = pe^{\lambda t} = p(e^{h\lambda})^n$, one root of (3.52) will approximate $e^{h\lambda}$ so that y_n approximates $y(t_n)$. That root will be called the "principle root" and will be denoted ξ_1. Other roots ξ_i, $i = 2, 3, \ldots, n$, which also give rise to solutions $p\xi_i$, will be called "extraneous roots." The size of extraneous roots affects the stability of the multi-value method, a topic which will be discussed later.

The principle root ξ_1 of Equation (3.52) approximates $e^{h\lambda}$. Assume a root of the form

$$\xi_1 = e^{h\lambda} + \gamma$$

where γ is small. To estimate the behavior of γ as a function of h, we have

$$\begin{aligned} 0 &= \rho(\xi_1) + h\lambda\sigma(\xi_1) \\ &= \rho(e^{h\lambda} + \gamma) + h\lambda\sigma(e^{h\lambda} + \gamma) \\ &= \rho(e^{h\lambda}) + \gamma\rho'(e^{h\lambda}) + 0(\gamma^2) + h\lambda\sigma(e^{h\lambda}) + 0(h\gamma) \\ &= \rho(e^{h\lambda}) + \gamma\rho'(e^{h\lambda}) + h\lambda\sigma(e^{h\lambda}) + 0(\gamma^2 + h\gamma). \end{aligned} \tag{3.54}$$

In view of (3.23), (3.54) becomes

$$0 = C_{r+1}(h\lambda)^{r+1} + \gamma\rho'(e^{h\lambda}) + 0(h^{r+2}) + 0(\gamma^2 + \gamma h).$$

Now,

$$\rho'(\xi) = \sum_{i=0}^{k-1} \alpha_i (k-i)\xi^{k-i-1}.$$

Note from Equation (3.26) that if $r \geq 1$, $\rho'(1) = -1$. Therefore

$$\rho'(e^{h\lambda}) = \rho'(1+0(h))$$

$$= \sum_{i=0}^{k-1} \alpha_i(k-i)\,[1 + 0(h)]^{k-i-1}$$

$$= \sum_{i=0}^{k-1} \alpha_i(k-i) + 0(h)$$

$$= \rho'(1) + 0(h)$$

$$= -1 + 0(h).$$

Thus, Equation (3.55) becomes

$$0 = C_{r+1}(h\lambda)^{r+1} - \gamma + 0(h^{r+2}) + 0(\gamma^2 + 2\gamma h). \tag{3.56}$$

We only want the aysmptotic behavior of γ for small γ as $h \to 0$. Hence, since γ is small the term $0(\gamma^2 + 2\gamma h)$ in Equation (3.56) will be truncated. Solving for γ in Equation (3.56) yields

$$\gamma = C_{r+1}(h\lambda)^{r+1} + 0(h^{r+2}).$$

So Equation (3.53) becomes

$$\xi_1 = e^{h\lambda} + C_{r+1}(h\lambda)^{r+1} + 0(h^{r+2}). \tag{3.57}$$

Therefore, ξ_1 approximates $e^{h\lambda}$ to order h^{r+1}.

In Chapter 1 stability of a multivalue method was defined as the boundedness of the effects of a perturbation in the starting values for all $0 < h \leq h_o$. To study these effects, consider the difference, e_n, between the numerical solution of the differential equation $y' = \lambda y$ and the actual solution of $y' = \lambda y$ [see Equation (3.6)]. It then follows from Equation (3.1) that

$$0 = \sum_{i=0}^{k} \alpha_i \left(y_{n-i} - y(t_{n-i}) \right) + h\beta_i \lambda \left(y_{n-i} - y(t_{n-i}) \right)$$

$$= \sum_{i=0}^{k} (\alpha_i + h\lambda\beta_i) e_{n-i}. \tag{3.58}$$

We now look for solutions of the form $e_n = p\,\xi^n$, p a constant, where the ξ are roots of

$$0 = \sum_{i=0}^{k} (\alpha_i + h\lambda\beta_i)\,\xi^{k-i}$$

$$= \rho(\xi) + h\lambda\sigma(\xi). \tag{3.59}$$

If all the roots ξ_j, $j = 1, 2, \ldots, k$ of (3.59) are distinct, the general solution of (3.58) is

$$e_n = \sum_{j=1}^{k} p_j\,\xi_j^n \tag{3.60}$$

where the p_j are constants. If some of the roots are equal, then this must be modified. For example, if ξ_i is an m-fold root of (3.59), then the term

$$(p_i + p_{i+1}n + p_{i+2}n^2 + \ldots + p_{i+m-1}n^{m-1})\,\xi_i^n$$

will occur.

If any $|\xi_j| > 1$, then e_n grows exponentially. Thus, the method is not absolutely stable for that $h\lambda$. If we are interested in an unbounded range of t, then the problem will be unstable. If any $|\xi_j| = 1$ where ξ_j is a m-fold root, $m > 1$, then the method is not stable. Therefore, to have any kind of stability, we will require all $|\xi_j| \leq 1$ where if $|\xi_j| = 1$, then that ξ_j is a simple root of $\rho(\xi) + h\lambda\sigma(\xi) = 0$.

The solutions of (3.59) are functions of $h\lambda$, that is, $\xi_i = \xi_i(h\lambda)$. The roots of a polynomial are continuous functions of its coefficients. Therefore, if $|\xi_i(0)| < 1$, there exists an h_o for any fixed λ such that $|\xi_i(h\lambda)| \leq 1$ where $h \leq h_o$. If there are some simple roots ξ_i such that $|\xi_i(0)| = 1$, then

$$\xi_i(h\lambda) = \xi_i(0) + 0(h)$$

by a Taylor's series expansion about zero where h is sufficiently small. [The roots of (3.59) are differentiable functions of $h\lambda$ in any region of $h\lambda$ where they are distinct.] Hence,

$$\left|\xi_i^n(h\lambda)\right| \leq \left|\xi_i(0) + 0(h)\right|^n$$

$$\leq \left|\xi_i(0) + kh\right|^n$$

$$\leq (1+kh)^n$$

$$\leq e^{khn}$$

$$\leq e^{kt}$$

for $t \leq b$ and k some constant (note that the bound is independent of h). Thus, a change in the starting values by a fixed amount produces a bounded change in the numerical solution for all $0 < h \leq h_o$. Hence, by Definition 1.2, the multivalue method is stable. In fact, the multivalue method is absolutely stable for those $h\lambda$ where $\left|\xi\right| \leq 1$; if $\left|\xi\right| = 1$, then that ξ is simple (see Definition 1.4).

From what was done in the preceding paragraph, we suspect that the roots of $\rho(\xi) = 0$ must obey some such condition for stability. Recall that convergence for a multivalue method was defined to mean that any desired degree of accuracy can be achieved in solving (1.1) numerically by picking a small enough h. That is, as $h \rightarrow 0$, $y_n \rightarrow y(t_n)$. Thus, for a convergent multivalue method, we require some condition on the roots of $\rho(\xi) = 0$ [see Equation (3.1)] for stability. If the same analysis is done on the roots of $\rho(\xi) = 0$ that was done in the previous paragraph, we will find that the roots of $\rho(\xi) = 0$ must also lie in the unit circle. If they are on the unit circle, they must be simple. This condition is called the root condition and such $\rho(\xi)$ will be referred to as stable polynomials. This leads us to the following definitions for multivalue methods in solving $y' = \lambda y$ (see Gear [1, pp. 125-126]):

Definition 3.2

A multivalue method is strongly stable if all roots of $\rho(\xi) = 0$ are inside the unit circle except for the root $\xi = 1$ (such stability is often referred to as Dahlquist stability).

Definition 3.3

A multivalue method is weakly stable if it is stable but has more than one root on the unit circle.

The behavior of a multivalue method that is not stable is seen in the following example of a 2-step third order formula:

$$y_n = -4y_{n-1} + 5y_{n-2} + 4hf_{n-1} + 2hf_{n-2}.$$

If the equation $y' = 0$ is solved with initial values $y_0 = 0$, $y_1 = \epsilon$, we get the following results [note that $\rho(\xi) = \xi^2 + 4\xi - 5$ or $\rho(\xi) = (\xi + 5)$ $(\xi - 1)$]:

Table 3.1. Effect of instability

n	y
0	0
1	ϵ
2	-4ϵ
3	21ϵ
4	-104ϵ
5	521ϵ
6	-2604ϵ

This behavior is independent of h so it is evident that there is no hope for the computed solution to converge to the true solution $y(t_i) = 0$, $i = 1, 2, \ldots, N$ as $h \to 0$.

Suppose that we look at the stability of the 3-step third order Adams-Bashforth method defined by (1.5) in solving $y' = \lambda y$. A solution of the form $y_n = p\xi^n$ can be found if ξ is a root of Equation (3.59). The polynomials ρ and σ for this method are

$$\rho(\xi) = \xi^3 - \xi^2 = \xi^2(\xi - 1) \tag{3.61}$$

$$\sigma(\xi) = -\frac{1}{12}(23\xi^2 - 16\xi + 5). \tag{3.62}$$

One of the roots of $\rho(\xi) = 0$ is $\xi = 1$ while another root is a double root which is at the center of the unit circle. Therefore, by Definition 3.2 the 3-step Adams-Bashforth method of order three is strongly stable. If $h = 1/8$ and $\lambda = 1$, Equation (3.59) is

$$\xi^3 - \frac{73}{96}\xi^2 - \frac{16}{96}\xi + \frac{5}{96} = 0. \tag{3.63}$$

Hence,

$$\left|\xi^3\right| = \frac{1}{96}\left|73\xi^2 + 16\xi - 5\right|$$

$$\leq \frac{1}{96}\left(73\left|\xi^2\right| + 16\left|\xi\right| + 5\right)$$

$$\leq \frac{94}{96}\max\left\{\left|\xi^2\right|, 1\right\}$$

which implies that

$$\left|\xi\right| < 1.$$

So all the roots of Equation (3.63) are inside the unit circle. Therefore, small perturbations in the initial value will not cause large errors in later steps. On the other hand, if $\lambda = -100$ and h remains the same Equation (3.59) becomes

$$\xi^3 + \frac{2204}{96}\xi^2 - \frac{1600}{96}\xi + \frac{500}{96} = 0. \qquad (3.64)$$

If ξ_1, ξ_2, and ξ_3 are roots of Equation (3.64), then Equation (3.64) can be written as

$$0 = (\xi - \xi_1)(\xi - \xi_2)(\xi - \xi_3)$$

$$= \xi^3 - (\xi_1 + \xi_2 + \xi_3)\xi^2 + (\xi_1\xi_2 + \xi_1\xi_3 + \xi_2\xi_3)\xi - \xi_1\xi_2\xi_3.$$

Equating coefficients of ξ^2 yields

$$\xi_1 + \xi_2 + \xi_3 = -\frac{2204}{96}.$$

Thus,

$$\frac{2204}{96} = \left|\xi_1 + \xi_2\ \xi_3\right|$$

$$\leq \left|\xi_1\right| + \left|\xi_2\right| + \left|\xi_3\right|$$

$$\leq 3\max\left\{\left|\xi_1\right|\right\} \quad 1 \leq i \leq 3.$$

Hence, it follows that one root of (3.64) will exceed $\frac{1}{3}(\frac{2204}{96}) >> 1$ in absolute value, so small perturbations will be magnified rapidly. So our choice of h is too large. We have already seen that the 3-step Adams-Bashforth method of order three is strongly stable [see Equations (3.61) and (3.62)]. Hence, since the roots of $\rho(\xi) + h\lambda\sigma(\xi) = 0$ depend continuously on $h\lambda$ and are the roots of $\rho(\xi)$ when $h = 0$, there exists a region about $h\lambda = 0$ where the method is absolutely stable. So, if h is chosen so that $h\lambda$ lies within this region, then small perturbations in the initial value will not cause large errors in later steps in solving $y' = -100y$.

Suppose now that $Re(\lambda) > 0$ [recall that the solution of $y' = \lambda y$ is $y = p(e^{h\lambda})^n$]. Since $|\xi_1| \approx |e^{\lambda h}| > 1$ [see Equation (3.57)], absolute stability of the multivalue method is not required. This must be so so that the principle root ξ_1 of Equation (3.59) will track $e^{h\lambda}$. So that the numerical approximation is reasonable, we must require all extraneous roots of Equation (3.59) to be less than the principle root in absolute value.

As has been seen, h must be chosen so that the perturbations due to solutions of (3.59) do not grow faster than the solution which is $pe^{\lambda t}$ (note that for $\lambda = \lambda_1 + i\lambda_2$, $pe^{\lambda t} = pe^{\lambda_1 t}\cos\lambda_2 t + ipe^{\lambda_1 t}\sin\lambda_2 t$) for general starting conditions. If $Re(\lambda) \leq 0$, no root of (3.59) should exceed 1 in absolute value, whereas if $Re(\lambda) > 0$, the principle root will approximate $e^{h\lambda}$ and none of the extraneous roots should be larger than the principle root in absolute value. This leads to definitions of absolute and relative stability for the test equation $y' = \lambda y$:

Definition 3.4

A multivalue method is absolutely stable for those values of $h\lambda$ where roots of (3.59) are inside the unit circle or simple on the unit circle.

Definition 3.5

A multivalue method is relatively stable where the extraneous roots of (3.59) are less than the principle root in absolute value.

If $Re(\lambda) > 0$, then h must be chosen so that $h\lambda$ lies outside the region of absolute stability so that $|\xi_1| > 1$.

Let us look at absolute stability regions for the Adams-Bashforth predictor multivalue methods of orders one through six and the Adams-Moulton corrector multivalue methods of orders one through six in solving the test equation $y' = \lambda y$, $Re(\lambda) \leq 0$. [The larger the region, the larger h can be made within the truncation error restriction.] For absolute stability, the roots of (3.59) must be inside the unit circle or simple on the unit circle by Definition 3.4. For the Adams-Bashforth 1-step first order method, it follows from Table 3.2 and Equations (3.19) and (3.20) that

$$\rho(\xi) = \xi - 1$$

$$\sigma(\xi) = -1.$$

Table 3.2. Adams-Bashforth methods

Order	Method
1	$y_n = y_{n-1} + hf_{n-1}$
2	$y_n = y_{n-1} + \frac{h}{2}(3f_{n-1} - f_{n-2})$
3	$y_n = y_{n-1} + \frac{h}{12}(23f_{n-1} - 16f_{n-2} + 5f_{n-3})$
4	$y_n = y_{n-1} + \frac{h}{24}(55f_{n-1} - 59f_{n-2} + 37f_{n-3} - 9f_{n-4})$
5	$y_n = y_{n-1} + \frac{h}{720}(1901f_{n-1} - 2774f_{n-2} + 2616f_{n-3} - 1274f_{n-4} + 251f_{n-5})$
6	$y_n = y_{n-1} + \frac{h}{1440}(4277f_{n-1} - 7923f_{n-2} + 9982f_{n-3} - 7298f_{n-4} + 2877f_{n-5} - 475f_{n-6})$

Table 3.3. Adams-Moulton methods

Order	Method
1	$y_n = y_{n-1} + hf_n$
2	$y_n = y_{n-1} + \frac{h}{2}(f_n + f_{n-1})$
3	$y_n = y_{n-1} + \frac{h}{12}(5f_n + 8f_{n-1} - f_{n-2})$
4	$y_n = y_{n-1} + \frac{h}{24}(9f_n + 19f_{n-1} - 5f_{n-2} + f_{n-3})$
5	$y_n = y_{n-1} + \frac{h}{720}(251f_n + 646f_{n-1} - 264f_{n-2} + 106f_{n-3} - 19f_{n-4})$
6	$y_n = y_{n-1} + \frac{h}{1440}(475f_n + 1427f_{n-1} - 798f_{n-2} + 482f_{n-3}$ $-173f_{n-4} + 27f_{n-5})$

Thus, Equation (3.59) becomes

$$\xi - (1 + h\lambda) = 0.$$

Therefore,

$$1 \geq \left| \xi \right| = \left| 1 + h\lambda \right|$$

which implies that the Adams-Bashforth 1-step first order method will be absolutely stable for those $h\lambda$ where

$$\left| 1 + h\lambda \right| \leq 1.$$

This is a circle in the complex $h\lambda$-plane of radius 1 centered at $h\lambda = -1$. When the same thing is done for the 1-step first order Adams-Moulton method it follows that the region of absolute stability is all $h\lambda$ where

$$\left| 1 - h\lambda \right| \geq 1.$$

This is the exterior of a circle of radius 1 centered at $h\lambda = 1$. Since we are interested in $Re(\lambda) < 0$, we restrict our region of absolute stability to be in the negative half plane.

For the 1-step second order Adams-Mounton method, we find that

$$\rho(\xi) = \xi - 1$$

$$\sigma(\xi) = -\frac{1}{2}\xi - \frac{1}{2}.$$

Hence, Equation (3.59) becomes

$$(1 - \frac{h\lambda}{2})\xi - (1 + \frac{h\lambda}{2}) = 0.$$

Solving for ξ, it follows that

$$\xi = \frac{2 + h\lambda}{2 - h\lambda}.$$

For absolute stability,

$$\left|\xi\right| = \left|\frac{2 + h\lambda}{2 - h\lambda}\right| \leq 1.$$

The last inequality holds for those $h\lambda$ which lie in the negative half plane. Thus, the negative half plane is the region of absolute stability for the 1-step second order Adams-Moulton method.

To find regions of absolute stability of multivalue methods of higher order involves a little more work. Consider the 3-step Adams-Bashforth method of order three [see Equation (1.5)]. Using Equations (3.61) and (3.62), Equation (3.59) becomes

$$\xi^3 - (1 + \frac{23}{12}\mu)\xi^2 + \frac{16}{12}\mu\xi - \frac{5}{12}\mu = 0 \qquad (3.65)$$

where $\mu = h\lambda$. Solving for μ yields

$$\mu = \frac{12\xi^2(1-\xi)}{-23\xi^2 + 16\xi - 5} = f(\xi) \qquad (3.66)$$

which is analytic on the unit circle $|\xi| = 1$ and its interior except at the poles $\xi = .087 \pm .4581i$ which lie inside the unit circle $|\xi| < 1$. Let Γ represent the circle $|\xi| = 1$ in the ξ − plane having a positive orientation. Since f [see Equation (3.66)] is analytic on Γ, then f (Γ) is a closed curve in the μ-plane.

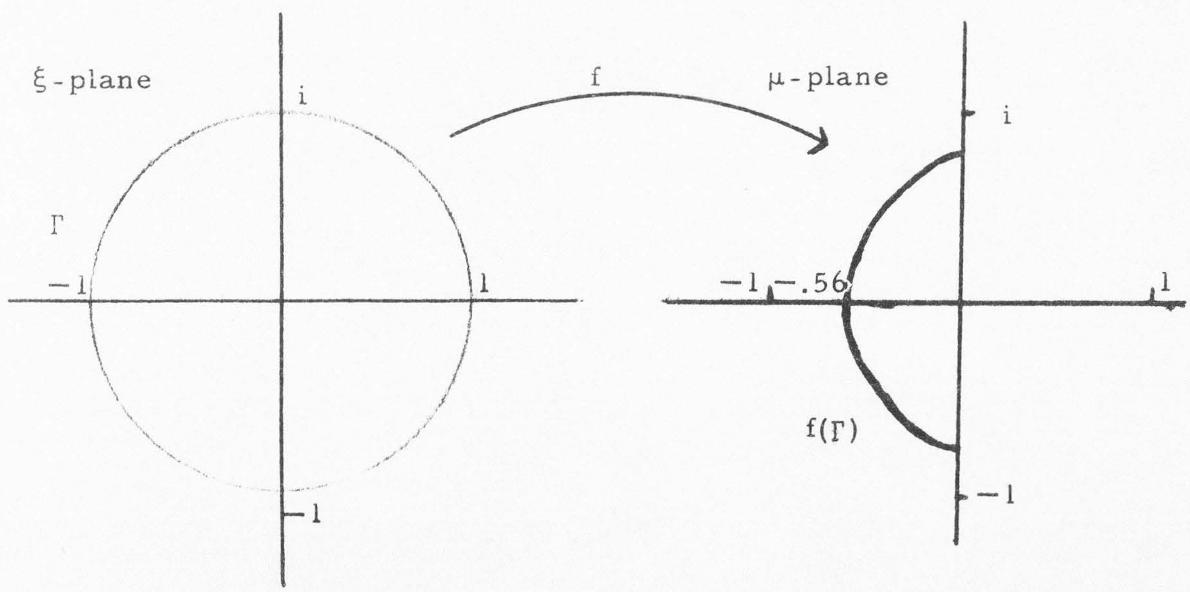

Figure 3.1. Region of absolute stability for the 3-step Adams-Bashforth method of order three.

There are three zeros in Equation (3.65) [a simple zero is counted once, a double zero twice, a triple zero three times, etc.]. Therefore, looking at Equation (3.66), for each μ in the range of f there exist three ξ's [these ξ's are zeros of Equation (3.65)] in the domain of f that map to that μ under this mapping. For absolute stability, we require these ξ's to be inside the unit circle or simple on the unit circle. Hence, let $|\xi| \leq 1$ be the domain of f. Then the image of f where $Re(\mu) \leq 0$ will be the region of absolute stability. The curve $f(\Gamma)$, $Re(\mu) < 0$ is shown in Figure 3.1.

We will now show that the interior of $f(\Gamma)$ where $Re(\mu) \leq 0$ (see Figure 3.1) is the region of absolute stability for the 3-step Adams-Bashforth method of order three. To do this, we must show that for every μ contained in the interior of $f(\Gamma)$ there exist three ξ's in the domain of f that map to that μ (recall that $|\xi| \leq 1$ is the domain of f). We will use the "Argument Principle" which we will state without proof (see Flanigan [2, p. 278]):

Theorem 3.5 (The Argument Principle)

Let Γ be a piecewise-smooth positively oriented simple closed curve in the ξ-plane, and let f be analytic and nonconstant on a domain containing Γ and its interior, except perhaps for a finite number of poles strictly inside Γ. Let μ_o be a point of the μ-plane not on the curve $f(\Gamma)$. Also, let $N\mu_o(\Gamma)$ represent the number of points ξ in the interior of Γ such that $f(\xi) = \mu_o$, $N_\infty(\Gamma)$ represent the number of poles of f strictly inside Γ, and $n(f(\Gamma); \mu_o)$ represent the number of times that $f(\Gamma)$ wraps around μ_o in the μ-plane. Then

$$N\mu_o(\Gamma) - N_\infty(\Gamma) = \frac{1}{2\pi i} \int_\Gamma \frac{f'(\xi)\, d\xi}{f(\xi) - \mu_o}$$

$$= n(f(\Gamma); \mu_o)$$

where $i = \sqrt{-1}$.

[The term $n(f(\Gamma); \mu_o)$ will be referred to as the winding number of $f(\Gamma)$ with respect to μ_o.] We will also state, without proof, the following lemma (see Flanigan [2, p. 275]):

Lemma 3.1

If Ω is a closed curve and μ_o, μ_1 are points in the same component (some open set) of $C - \Omega$ (where C is the complex plane), then they have the same winding number,

$$n(\Omega; \mu_1) = n(\Omega; \mu_o).$$

In this case, let Γ represent the positive oriented circle $|\xi| = 1$. Recall that f [see Equation (3.66)] is analytic on Γ and its interior except at the poles $\xi = .087 \pm .458i$ which lie inside Γ. Therefore, in this case $N_\infty(\Gamma) = 2$. Pick μ_o in the interior of $f(\Gamma)$, say $\mu_o = -1/3$ (see Figure 3.1). Then there are three ξ's strictly inside Γ such that $f(\xi) = -1/3$. These are $\xi_1 \sim .711$, $\xi_2 \sim -.65$, and $\xi_3 \sim .3$. Hence, $N\mu_o(\Gamma) = 3$. So it follows from Theorem 3.5 that

$$n(f(\Gamma); \mu_o) = N\mu_o(\Gamma) - N_\infty(\Gamma)$$

$$= 1.$$

Therefore, f wraps Γ around μ_o once as has been seen already from Figure 3.1. Let Ω represent $f(\Gamma)$. The set $C - \Omega$ obtained by removing Ω from the μ-plane breaks up into two components; each of which is open and disjoint from the other (one inside component and one outside component). Pick $\mu \neq \mu_o$, $Re(\mu) \leq 0$ so that μ and μ_o are in the same component of $C - \Omega$. Then by Lemma 3.1

$$N_\mu(\Gamma) - N_\infty(\Gamma) = n(\Omega; \mu)$$

$$= n(\Omega; \mu_o)$$

$$= n(f(\Gamma); \mu_o)$$

$$= 1$$

which implies that $N_{\mu}(\Gamma) = 3$ since $N_{\infty}(\Gamma) = 2$. Hence, for every μ contained in the interior of $f(\Gamma)$ there exist three ξ's contained in the interior of Γ such that $f(\xi) = \mu$. Therefore, the region of absolute stability consists of the region $f(\Gamma)$ and the interior of $f(\Gamma)$ where $Re(\mu) \leq 0$.

The above technique can be used to find the regions of absolute stability for the rest of the Adams-Bashforth-Moulton multivalue methods. Figures 3.2 and 3.3 depict these regions.

The mapping f is different for each method. When the poles of f are computed for each method, it is found that the poles of f corresponding to the Adams-Bashforth methods all lie inside the unit circle whereas the poles of f corresponding to the Adams-Moulton methods lie inside the unit circle except for one. In finding the regions of absolute stability for each method, $f(\Gamma)$ was found. Then a μ_o in the μ-plane was picked so that μ_o was contained in the interior of $f(\Gamma)$. Then ξ was found inside the interior of Γ where $f(\xi) = \mu_o$ to insure us that such ξ do exist inside the unit circle. Tables 3.4 and 3.5 depict the poles of each transformation, the μ_o that was picked and the ξ that are associated with that μ_o (see Figures 3.2 and 3.3). The numbers are all rounded to the number of the figure shown. We see from Tables 3.4 and 3.5 that

$$n(f(\Gamma); \mu_o) = N\mu_o(\Gamma) - N_{\infty}(\Gamma)$$

$$= 1$$

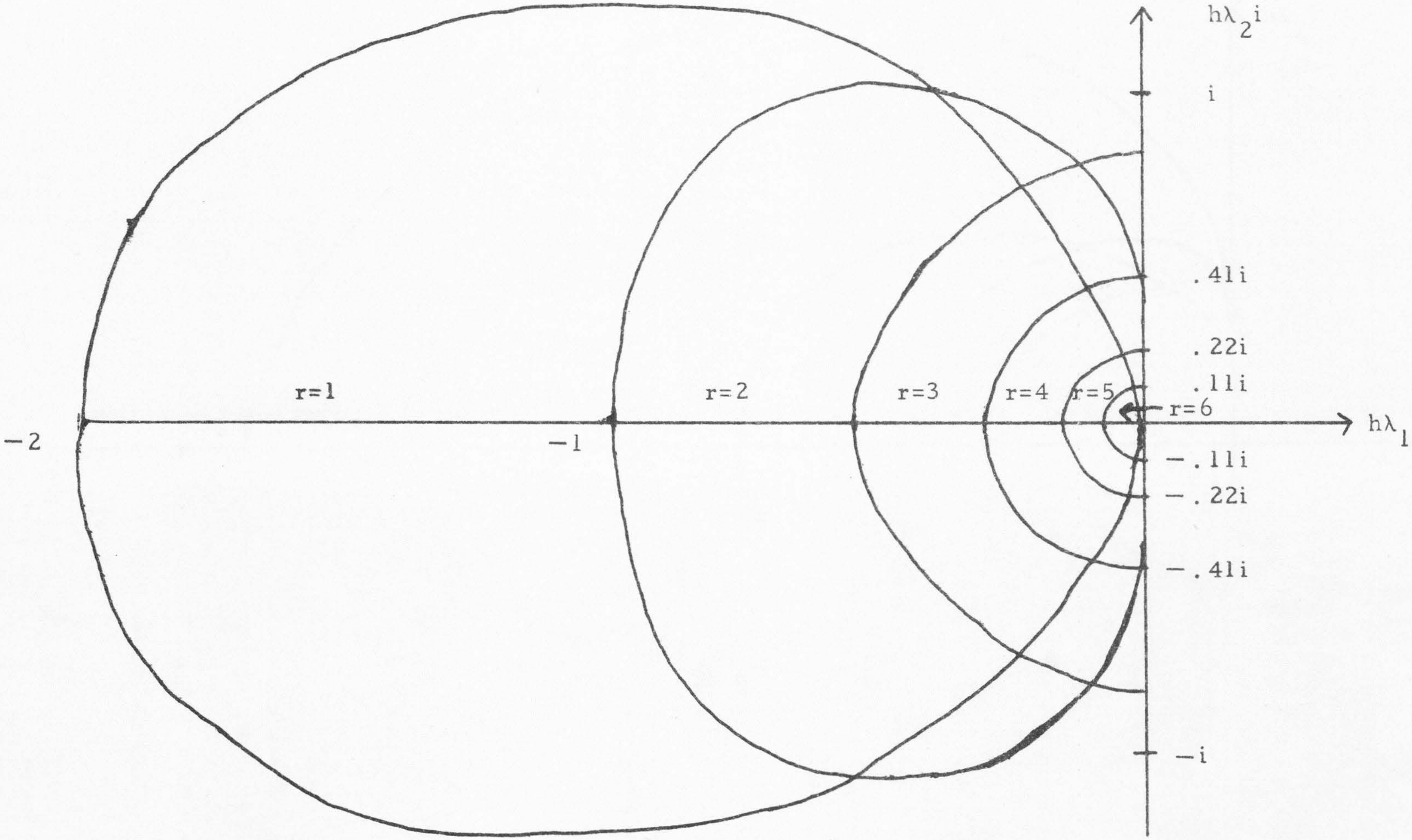

Figure 3.2. Stability regions for Adams-Bashforth methods. Method of order r=k is stable inside region indicated left of origin.

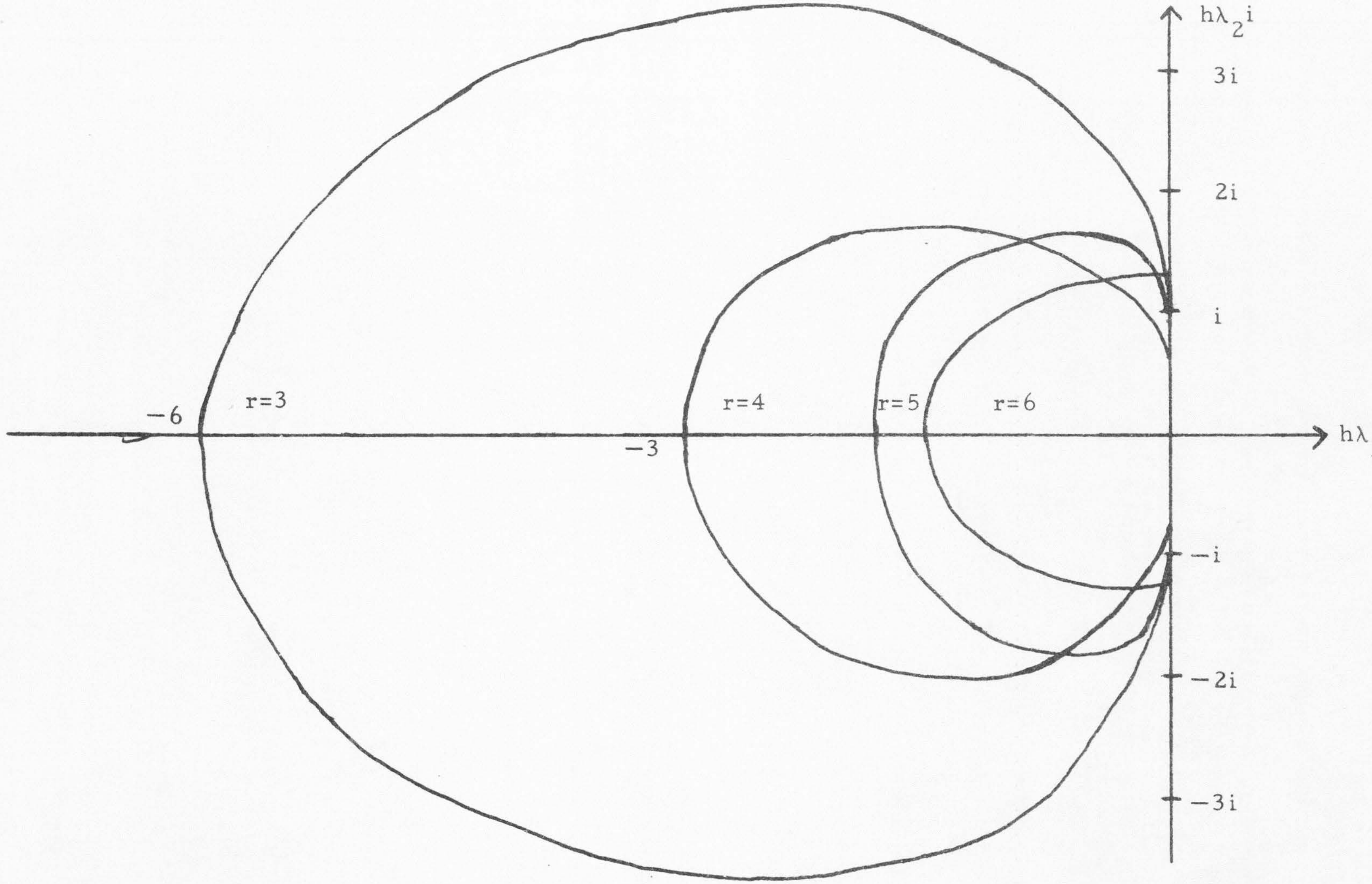

Figure 3.3. Stability regions for Adams-Moulton methods. Method of order r=k+1 is stable inside region indicated.

Table 3.4. Adams-Bashforth methods

Order	Transformation	Poles	ξ	μ_o	$N_\infty(\Gamma)$	$N_\mu(\Gamma)$
2	$f(\xi) = \dfrac{2\xi(1-\xi)}{-3\xi+1}$	$-.333$	$.64, -.39$	$-.5$	1	2
3	$f(\xi) = \dfrac{12\xi^2(1-\xi)}{-23\xi^2+16\xi-5}$	$.087 \pm .458i$	$.3, -.65, .71$	$-.33$	2	1
4	$f(\xi) = \dfrac{24\xi^3(1-\xi)}{-55\xi^3+59\xi^2-37\xi+9}$	$.333 \pm .539i$ $.407$	$.268 \pm .252i$ $.78, -.888$	$-.25$	3	4
5	$f(\xi) = \dfrac{720\xi^4(1-\xi)}{-1901\xi^4+2774\xi^3-2616\xi^2+1274\xi-251}$	$.417 \pm .17i$ $.313 \pm .744i$	$.172 \pm .384i$ $.882, .319$ $.876$	$-.125$	4	5
6	$f(\xi) = \dfrac{1440\xi^5(1-\xi)}{-4277\xi^5+7923\xi^4-9982\xi^3+7298\xi^2-2877\xi+475}$	$.292 \pm .938i$ $.417 \pm .301i$ $.435$	$.303 \pm .14$ $.783 \pm .479$ $.936, -.896$	$-.066$	5	6

Table 3.5. Adams-Moulton methods

Order	Transformation	Poles	ξ	μ_o	$N_\infty(\Gamma)$	$N\mu_o(\Gamma)$
3	$f(\xi) = \dfrac{12\xi(1-\xi)}{-5\xi^2 - 8\xi + 1}$	.117, −1.717	−.623, .178	−3	1	2
4	$f(\xi) = \dfrac{24\xi^2(1-\xi)}{-9\xi^3 - 19\xi^2 + 5\xi - 1}$	.127 ± .175i −2.366	.204 ± .15 −.741	−2	2	3
5	$f(\xi) = \dfrac{720\xi^3(1-\xi)}{-251\xi^4 - 646\xi^3 + 264\xi^2 - 106\xi + 19}$	.087 ± .321i .23, −2.977	.173 ± .216 .387, −.658	−1	3	4
6	$f(\xi) = \dfrac{1440\xi^4(1-\xi)}{-475\xi^5 - 1427\xi^4 + 798\xi^3 - 482\xi^2 + 173\xi - 27}$	.248 ± .128i .032 ± .452i −3.564	.34 ± .514 .116 ± .344 −.905	−1	4	5

for every transformation f. Using the same argument used in the last paragraph, if μ is picked from the interior of $f(\Gamma)$ where $\mu \neq \mu_o$, then by Lemma 3.1

$$\begin{aligned} N_\mu(\Gamma) - N_\infty(\Gamma) &= n(f(\Gamma); \mu) \\ &= n(f(\Gamma); \mu_o) \\ &= 1. \end{aligned}$$

Hence, for every transformation f there exist ξ_i contained in the interior of Γ, $i = 1, 2, \ldots, r$ such that $f(\xi_i) = \mu$ for every μ contained in the interior of $f(\Gamma)$ where $r = k$ for a kth order Adams-Bashforth method and $r = k-1$ for a kth order Adams-Moulton method. Therefore, by finding $f(\Gamma)$, the region of absolute stability lies in the interior of $f(\Gamma)$ where $Re(\mu) \leq 0$.

Suppose we now look at the most general 3-step multivalue method having the form

$$\begin{aligned} &\alpha_o y_n + \alpha_1 y_{n-1} + \alpha_2 y_{n-2} + \alpha_3 y_{n-3} + h\beta_o f_n + h\beta_1 f_{n-1} \\ &\qquad + h\beta_2 f_{n-2} + h\beta_3 f_{n-3} = 0. \qquad (3.67) \end{aligned}$$

In solving for the α's and β's we want to make sure that the method will be strongly stable. So we will try to find that region where it will be strongly stable. If we require (3.67) to have fourth order, then by (3.4) the α's and β's must satisfy the five equations

$$
\begin{aligned}
&\alpha_o + \alpha_1 + \alpha_2 + \alpha_3 &&= 0 \\
&\alpha_1 + 2\alpha_2 + 3\alpha_3 - \beta_o - \beta_1 - \beta_2 - \beta_3 &&= 0 \\
&\alpha_1 + 4\alpha_2 + 9\alpha_3 \qquad - 2\beta_1 - 4\beta_2 - 6\beta_3 &&= 0 \\
&\alpha_1 + 8\alpha_2 + 27\alpha_3 \qquad - 3\beta_1 - 12\beta_2 - 27\beta_3 &&= 0 \\
&\alpha_1 + 16\alpha_2 + 81\alpha_3 \qquad - 4\beta_1 - 32\beta_2 - 108\beta_3 &&= 0.
\end{aligned}
$$

By Equation (3.18), $\sigma(1) = 1$ from which the additional equation

$$\beta_o + \beta_1 + \beta_2 + \beta_3 = 1$$

is obtained. These six equations in eight unknowns can be solved in terms of two free parameters, say β_2 and β_3. Therefore,

$$\alpha_o = \frac{1}{24}(-17 + 30\beta_2 - 18\beta_3)$$

$$\alpha_1 = \frac{1}{24}(9 - 54\beta_2 + 90\beta_3)$$

$$\alpha_2 = \frac{1}{24}(9 + 18\beta_2 - 126\beta_3)$$

$$\alpha_3 = \frac{1}{24}(-1 + 6\beta_2 + 54\beta_3)$$

$$\beta_1 = \frac{1}{24}(18 - 12\beta_2 - 36\beta_3)$$

$$\beta_o = 1 - \beta_1 - \beta_2 - \beta_3$$

while the error coefficient is given by

$$C_5 = \frac{1}{120}(1.5 - 5\beta_2 + 15\beta_3).$$

By Definition 3.2, (3.67) is strongly stable if all the roots of $\rho(\xi) = 0$ are inside the unit circle except for the root $\xi = 1$. So we want to find that region where this condition is satisfied. The polynomial $\rho(\xi)$ for this method is

$$\rho(\xi) = \frac{1}{24}\left[\xi^3(-17 + 30\beta_2 - 18\beta_3) + \xi^2(9 - 54\beta_2 + 90\beta_3) + \xi(9 + 18\beta_2 - 126\beta_3) + (-1 + 16\beta_2 + 54\beta_3)\right]$$

$$= \frac{1}{24}(\xi - 1)\left[\xi^2(-17 + 30\beta_2 - 18\beta_3) + \xi(-8 - 24\beta_2 + 72\beta_3) + (1 - 6\beta_2 - 54\beta_3)\right]. \quad (3.68)$$

One root of $\rho(\xi) = 0$ is $\xi = 1$. We are now interested in those values of β_2 and ρ_3 for which the quadratic factor in Equation (3.68) has roots inside the unit circle. The easiest way to find this is to find the boundary where $|\xi| = 1$ is a root. We find that $\xi = -1$ is a root of

$$(-17 + 30\beta_2 - 18\beta_3)\xi^2 + (-8 - 24\beta_2 + 72\beta_3) + (1 - 6\beta_2 - 54\beta_3) = 0 \quad (3.69)$$

[see Equation (3.68)] if $\beta_2 - 3\beta_3 = 1/6$. The value $\xi = 1$ is not a root of (3.69) for any finite values of β_2 and β_3 since the sum of the coefficients of Equation (3.69) is -24. The only other possibility is that a complex conjugate pair of ξ values occur on the unit circle. For this the coefficients of ξ^2 and 1 in Equation (3.66) must be equal [since if ξ_1 is a complex root such that $|\xi_1| = 1$ and $\bar{\xi}_1$ is its conjugate, then

$$\frac{1 - 6\beta_2 - 54\beta_3}{-17 + 30\beta_2 - 18\beta_3} = \xi_1 \bar{\xi}_1 = |\xi_1|^2 = 1$$

which implies that $1 - 6\beta_2 - 54\beta_3 = -17 + 30\beta_2 - 18\beta_3$] and the discriminant must be negative. This occurs when $\beta_2 + \beta_3 = 1/2$ and $108(\beta_2 + \beta_3)^2 \leq 12(\beta_2 + 33\beta_3) - 11$. This is the section of the line $\beta_2 + \beta_3 = 1/2$ where $\beta_2 \leq 5/12$. The line along which one extraneous root is zero is given by

$$1 - 6\beta_2 - 54\beta_3 = 0$$

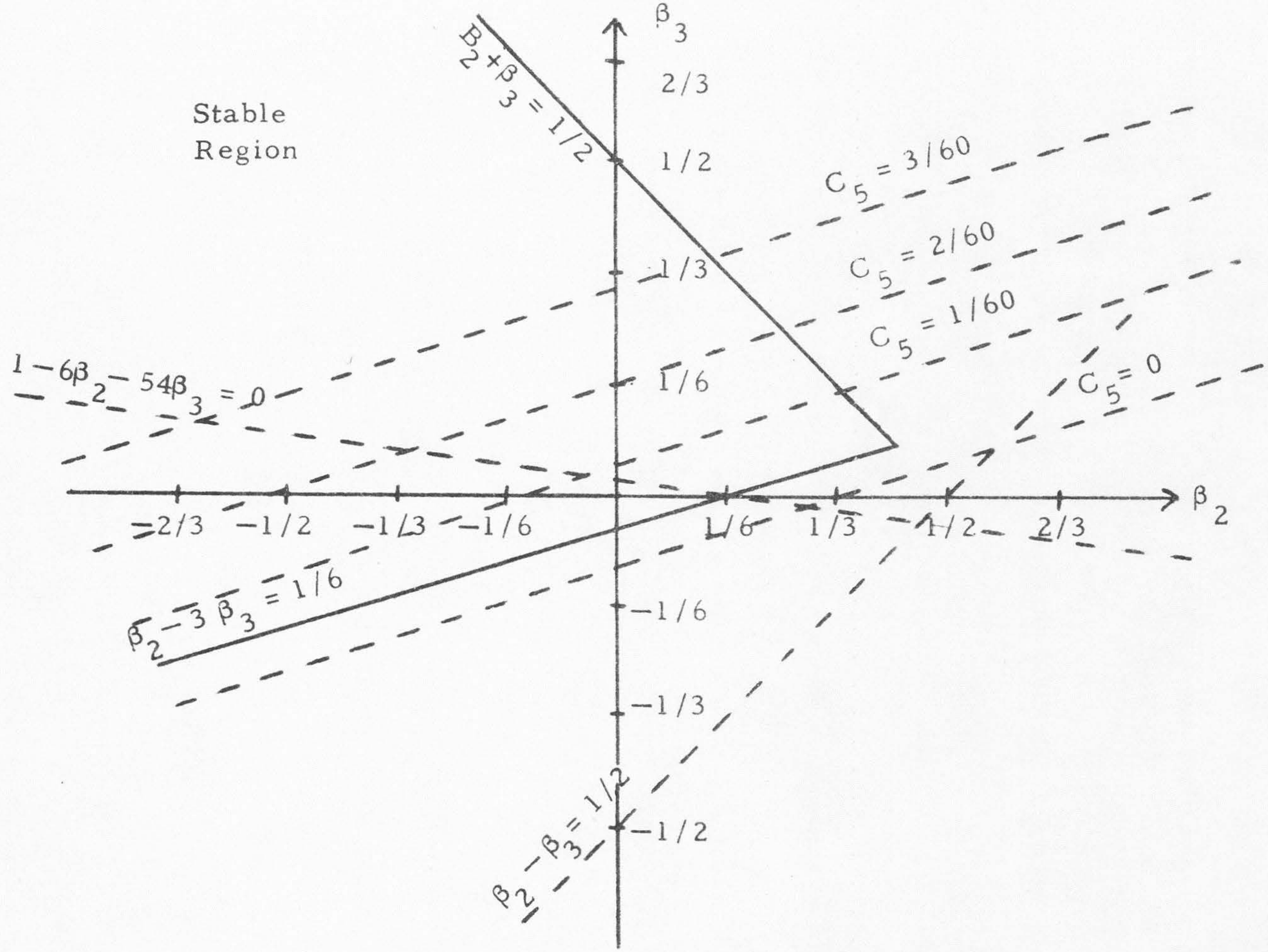

Figure 3.4. Values of β_2 and β_3 for which 3-step multivalue methods of order four are strongly stable.

while at $\beta_2 = -5/24$, $\beta_3 = 1/24$ both extraneous roots are zero. Figure 3.4 shows the region of strong stability in the (β_2, β_3)-plane and shows the lines of constant truncation error.

The line where the error coefficient is zero corresponds to a higher order method. It is outside of the stable region so a stable 3-step method cannot exceed order four. If the method is explicit, $\beta_o = 0$. Therefore, $0 = \beta_o = 1 - (\beta_1 + \beta_2 + \beta_3)$ which implies that $\beta_1 + \beta_2 + \beta_3 = 1$. Substituting $\beta_1 = \frac{1}{24}(18 - 12\beta_2 - 36\beta_3)$ into this last equation yields

$$\beta_2 - \beta_3 = 1/2.$$

This line is shown in Figure 3.4. The points found on this line yield an explicit multivalue method. However, this line is outside of the stable region so there does not exist a stable explicit 3-step fourth order multivalue method.

The truncation error coefficient is reduced by moving toward the line $\beta_2 - 3\beta_3 = 1/6$. However, this takes us toward a weakly stable method. It is not desirable either to move out too far to larger β_3 and smaller β_2 because large values affect the perturbation errors.

It is possible to put a bound on the maximum order of a stable multivalue method for first order equations. Recall that it is possible to pick ρ and σ (see page 60) so that order 2k could be achieved. We will now prove the following theorem:

Theorem 3.6

A stable k-step multivalue method for first order differential equations has maximum order

$$\begin{array}{ll} k+1 & \text{if } k \text{ is odd} \\ k+2 & \text{if } k \text{ is even.} \end{array}$$

An order of $k + 2$ can only occur if all roots of $\rho(\xi) = 0$ are on the unit circle.

Proof: Recall from Theorem 3.4 that a σ can be chosen for any ρ to make the order $k + 1$. Suppose that ρ is chosen so that it is stable. We introduce a new variable $z = x + iy$ by the linear fractional transformation

$$z = \frac{\xi - 1}{\xi + 1}, \qquad \xi = \frac{1 + z}{1 - z}.$$

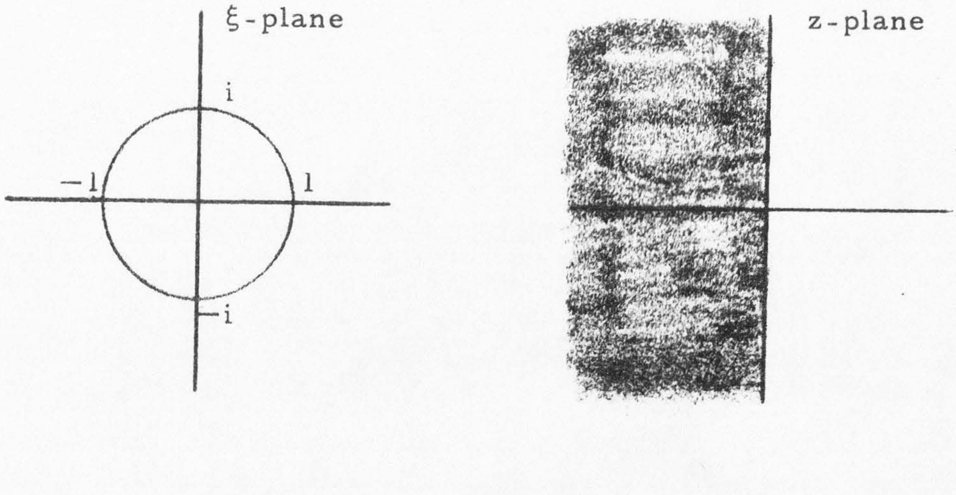

Figure 3.5. Mapping the unit circle onto the left half z-plane.

This transformation maps the disc $|\xi| < 1$ onto the half-plane $Re(z) < 0$, the circle $|\xi| = 1$ onto the imaginary axis, the point $\xi = i$ onto $z = 0$, the point $\xi = i$ onto $z = i$, and the point $\xi = -1$ onto $z = \infty$(see Figure 3.5). Define two new polynomials

$$R(z) = (\frac{1-z}{2})^k \quad \rho(\frac{1+z}{1-z}) \tag{3.70}$$

$$S(z) = (\frac{1-z}{2})^k \quad \sigma(\frac{1+z}{1-z}). \tag{3.71}$$

The polynomial ρ has degree $j \leq k$. Therefore,

$$R(z) = (\frac{1-z}{2})^k \rho(\frac{1+z}{1-z})$$

$$= (\frac{1-z}{2})^k \sum_{i=0}^{j} \alpha_i (\frac{1+z}{1-z})^{j-i}$$

$$= (\frac{1}{2})^k \sum_{i=0}^{j} \alpha_i \, (1+z)^{j-i} (1-z)^{k-j+1}.$$

If the same thing is done for $S(z)$, it follows that Equations (3.70) and (3.71) are both polynomials of degree k in z.

Our hypothesis is that ρ is stable. Consequently, all roots of R and ρ correspond except for when $\xi = -1$. This corresponds to the root of R at infinity, that is, the degree of R(z) decreases to k−1. Assume that the order of the multivalue method is r. The steps in the proof are as follows.

Solving for $\sigma(1+z)$ in Equation (3.24), it follows that

$$\sigma(1+z) = -\frac{\rho(1+z)}{\log(1+z)} + 0(z^r).$$

(Observe that $0(z^r) = C_{r+1}\, z^r$.) If we wet s(z) equal to terms in z^j $(0 \leq j \leq k-1)$ in the power series expansion of $-\rho(1+z)/\log(1+z)$, then $\sigma(\xi)$ can be found by writing

$$\sigma(\xi) = s(\xi-1).$$

Therefore,

$$\sigma(\xi) = -\frac{\rho(\xi)}{\log(\xi)} + 0\left((\xi-1)^r\right). \tag{3.72}$$

By substituting $\xi = \frac{z+1}{z-1}$ into Equation (3.72) and multiplying (3.72) by $\left(\frac{1-z}{2}\right)^k$, we get

$$\frac{R(z)}{\log\left(\frac{1+z}{1-z}\right)} + S(z) = 0(z^r). \tag{3.73}$$

The ξ corresponding to $z = 1$ is not a root of $\rho(\xi) = 0$ since ρ is stable. Hence, $z = 1$ is not a root or $R(z)$. So the term $R(z)/\log(\frac{1+z)}{1-z})$ in Equation (3.73) can be expanded in a power series in z, say $\sum_{n=0}^{\infty} v_n z^n$. Since $S(z)$ is of degree k, then $r \leq k+1$ or $k+2$ as k is odd or even if $v_n \neq 0$ for $n = k+1$ or $k+2$ as k is odd or even (note that if the multivalue method has order $r = k+1$ and $S(z) = \sum_{i=0}^{k} g_i z^i$, then $(v_o + g_o) = (v_1 + g_1) = \ldots = (v_k + g_k) = v_{k+1} = 0$). We will show that $v_n \neq 0$ for $n = k+1$ or $k+2$ as k is odd or even.

First, we will rewrite Equation (3.73) as

$$\frac{R(z)}{z} \cdot \frac{z}{\log(\frac{1+z}{1-z})} + S(z) = 0(z^r)$$

and look at the power series expansion of

$$\frac{R(z)}{z} \cdot \frac{z}{\log(\frac{1+z}{1-z})} . \tag{3.74}$$

Let $R(z) = c_o + c_1 z + \ldots c_k z^k$. Since $\xi = 1$ is a simple root of $\rho(\xi) = 0$, $z = 0$ is a simple root of $R(z) = 0$. Therefore, $c_o = 0$ and $c_1 \neq 0$. Without loss of generality, let $c_1 > 0$. Since ρ is a real polynomial, R is also real. Consequently, the roots of R are either real, x_δ, or occur in conjugate pairs, $x_\nu + iy_\nu$, where x_δ and $x_\nu \leq 0$, because roots of ρ

which are inside the unit circle or simple on the unit circle in the ξ-plane map into roots of R in the left half z-plane. By the factor theorem, R(z) can be written as

$$R(z) = c \prod (z - x_\delta) \prod (z - x_\nu - iy_\nu)(z - x_\nu + iy_\nu)$$

$$= c \prod (z + x_\delta) \prod (z^2 + 2z\,|x_\nu| + x_\nu^2 + y_\nu^2).$$

Therefore, every coefficient has the sign of c, but $c_1 > 0$, hence $c_i \geq 0,\ i \geq 2$.

Next consider

$$\frac{z}{\log\left(\frac{1+z}{1-z}\right)} = \frac{z}{2z + \frac{2z^3}{3} + \frac{2z^5}{5} + \ldots}$$

$$= \frac{1}{2 + \frac{2z^2}{3} + \frac{2z^4}{5} + \ldots}$$

$$= \sum_{\delta=0}^{\infty} h_{2\delta} z^{2\delta}. \qquad (3.75)$$

where h is a real constant. Observe that $h_o = 1/2$. Now, Equation (3.74) can be written as

$$\frac{R(z)}{z} \cdot \frac{z}{\log\left(\frac{1+z}{1-z}\right)} = \left(\sum_{i=1}^{k} c_i z^{i-1}\right)\left(\sum_{\delta=0}^{\infty} h_{2\delta} z^{2\delta}\right).$$

Recall that

$$\frac{R(z)}{z} \cdot \frac{z}{\log\left(\frac{1+z}{1-z}\right)} = \sum_{n=0}^{\infty} v_n z^n .$$

Therefore,

$$\sum_{n=0}^{\infty} v_n z^n = \left(\sum_{i=1}^{k} c_i z^{i-1}\right)\left(\sum_{\delta=0}^{\infty} h_{2\delta} z^{2\delta}\right) . \qquad (3.76)$$

It is our goal to show that $v_n \neq 0$ for $n = k+1$ or $n = k+2$ as k is odd or even. It follows from (3.76) that

$$v_{k+1} = h_2 c_k + h_4 c_{k-2} + \ldots + h_{k+1} c_1 \quad \text{for odd } k \qquad (3.77)$$

and

$$v_{k+1} = h_2 c_k + h_4 c_{k-2} + \dots + h_k c_2 \quad \text{for even } k. \tag{3.78}$$

We know that $c_1 > 0$, $c_j \geq 0$, $j > 2$. We will show that $h_{2\delta} < 0$, $\delta \geq 1$ (recall that $h_o = 1/2$) by considering the following lemma.

Lemma 3.1

If

$$\left(\sum_{n=0}^{\infty} d_n x^n\right)\left(\sum_{n=0}^{\infty} q_n x^n\right) = 1$$

where $d_n > 0$, $n \geq 0$ and $d_{n-1} \cdot d_{n+1} > d_n^2$, $n \geq 1$, then $q_n < 0$ for $n \geq 1$.

Proof: We set $d_o = 1$ without loss of generality. Therefore,

$$1 = (1 + d_1 x + d_2 x^2 + d_3 x^3 + \dots)(q_o + q_1 x + q_2 x^2 + q_3 x^3 + \dots)$$

$$= q_o + (q_o d_1 + q_1)x + (q_o d_2 + q_1 d_1 + q_2)x^2 + (q_o d_3 + q_1 d_2 + q_2 d_1 + q_3)x^3 + \dots$$

Equating terms in x^o on both sides of the equality sign, it follows that $q_o = 1$. If we examine the term in x^n, it follows that

$$0 = d_n + \sum_{k=1}^{n} d_{n-k} q_k . \tag{3.79}$$

By looking at the term in x^{n+1}, it follows that

$$0 = q_{n+1} + d_{n+1} + \sum_{k=1}^{n} d_{n+1-k} q_k$$

or

$$q_{n+1} = -d_{n+1} - \sum_{k=1}^{n} d_{n+1-n} q_k . \tag{3.80}$$

Multiplying (3.79) by d_{n+1}, (3.80) by d_n, and adding yields

$$d_n q_{n+1} = \sum_{k=1}^{n} q_k (d_{n+1} d_{n-k} - d_n d_{n+1-k}) . \tag{3.81}$$

Using the fact that $d_{n-1} \cdot d_{n+1} > d_n^2$, $n \geq 1$, it follows that

$$d_{n+1} d_n d_{n-1}^2 \cdots d_{n-k+2}^2 d_{n-k+1} d_{n-k} = (d_{n+1} d_{n-1})(d_n d_{n-2})$$

$$\cdots (d_{n-k+2} d_{n-k}) > d_n^2 d_{n-1}^2 \cdots d_{n-k+1}^2 \quad (3.83)$$

Therefore,

$$d_{n+1} d_{n-k} > d_n d_{n-k+1} \quad (3.84)$$

where we have divided both sides of (3.83) by

$$d_n d_{n-1}^2 d_{n-2}^2 \cdots d_{n-k+2}^2 d_{n-k+1} > 0 \quad (0 \leq k \leq n)$$

where $d_n > 0$, $n \geq 0$. So Equation (3.84) becomes

$$d_{n+1} d_{n-k} - d_n d_{n-k+1} > 0. \quad (3.85)$$

If $q_1, \ldots, q_n < 0$, then by (3.85) and the fact that $d_n > 0$, $n \geq 0$, Equation (3.81) shows that $q_{n+1} < 0$. Since

$$d_o q_1 + d_1 q_o = q_1 + d_1 = 0$$

$$q_1 = - d_1$$

$$< 0,$$

then the result is true for n = 1. Hence, by induction, $q_n < 0$ for $n \geq 1$.

Q. E. D.

Recall that [see Equation (3.75)]

$$\sum_{\delta=0}^{\infty} h_{2\delta} z^{2\delta} = \frac{1}{2 + \frac{2z^2}{3} + \frac{2z^4}{5} + \ldots}$$

$$= \frac{1}{\sum_{\delta=0}^{\infty} \left(\frac{2}{2\delta + 1} \right) z^{2\delta}}$$

Hence,

$$\left(\sum_{\delta=0}^{\infty} \frac{2}{(2\delta+1)} z^{2\delta} \right) \left(\sum_{\delta=0}^{\infty} h_{2\delta} z^{2\delta} \right) = 1.$$

Let $x = z^2$ and $d_n = 2/(2n+1)$ in Lemma 3.1. Then, since $d_n > 0$ for $n \geq 0$ and

$$d_{n-1} d_{n+1} = 4/(2n-1)(2n+3)$$

$$= 4/[(2n+1)^2 - 4]$$

$$\geq d_n^2$$

for $n \geq 1$, it follows that $h_{2\delta} = q_\delta < 0$ for $\delta \geq 1$.

Returning to Equation (3.77), since $c_1 > 0$, $c_j \geq 0$, $j \geq 2$, and $h_{2\delta} < 0$, $\delta \geq 1$, it follows that $v_{k+1} < 0$ for odd k, showing that k+1 is the maximum stable order. If k is even, then from (3.78) $v_{k+1} = 0$ only if $c_2 = c_4 = \ldots = c_k = 0$. In this case,

$$v_{k+2} = h_4 c_{k-1} + h_6 c_{k-3} + \ldots + h_{k+2} c_1 < 0,$$

so the maximum order is k+2, and it can be achieved by making $v_{k+1} = 0$ which requires that $c_2 = c_4 = \ldots = c_k = 0$ from (3.78). Since c_o is also zero, R(z) is an odd polynomial in z (recall that $R(z) = c_o + c_1 z + \ldots + c_k z^k$). Therefore, $R(-z) = -R(z)$. Consequently, roots of R(z) are also roots of R(−z), so that if $x_\nu + iy_\nu$ is a root of R(z) so is $-x_\nu - iy_\nu$. But, because of stability, both must be in the left half plane implying that $x_\nu = 0$, so that all roots of $R(z)$ are on the imaginary axis, which means that roots of $\rho(\xi) = 0$ are on the unit circle. Conversely, if the roots of $\rho(\xi) = 0$ are on the unit circle, those of $R(z)$ are on the imaginary axis, implying that $R(z)$ is odd and that $c_2 = c_4 = \ldots = c_k = 0$ so that the order is $k+2$ if the polynomial $\sigma(\xi)$ is chosen appropriately.

Q. E. D.

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